

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062624\
 Data File : BF138355.D
 Acq On : 26 Jun 2024 16:56
 Operator : CG\JU
 Sample : P2915-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-NORTH-1

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-BF061224.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138355.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	9	16	22	rVB	2356865	3046841	57.03%	7.863%
2	3.399	221	223	236	rBV	25052	62100	1.16%	0.160%
3	5.104	509	513	519	rVB	243672	298962	5.60%	0.772%
4	5.504	576	581	584	rBV	4161763	3852299	72.10%	9.942%
5	6.510	746	752	755	rBV	3846991	3918665	73.34%	10.114%
6	6.881	811	815	818	rBV	1425534	1195098	22.37%	3.084%
7	7.440	905	910	913	rBV	2751955	2624922	49.13%	6.775%
8	7.692	949	953	956	rBV	144606	112589	2.11%	0.291%
9	8.157	1028	1032	1036	rBV	1912736	1619590	30.31%	4.180%
10	8.469	1081	1085	1089	rBV	150351	144189	2.70%	0.372%
11	9.234	1210	1215	1218	rBV	6082602	5342887	100.00%	13.789%
12	9.910	1327	1330	1334	rVB	2159241	1938487	36.28%	5.003%
13	10.010	1342	1347	1357	rVB	251937	345981	6.48%	0.893%
14	10.704	1460	1465	1468	rBV	3366141	3285681	61.50%	8.480%
15	11.398	1579	1583	1586	rBV	2314109	1865732	34.92%	4.815%
16	11.922	1667	1672	1682	rBV2	575401	640182	11.98%	1.652%
17	12.098	1700	1702	1713	rVB4	32232	69992	1.31%	0.181%
18	12.704	1801	1805	1817	rBV	143578	188944	3.54%	0.488%
19	12.986	1848	1853	1856	rBV	5436463	4710835	88.17%	12.158%
20	13.098	1867	1872	1877	rBV2	39957	63941	1.20%	0.165%
21	13.880	2002	2005	2016	rVB	177640	254820	4.77%	0.658%
22	14.033	2025	2031	2035	rBV	1563346	1391859	26.05%	3.592%
23	14.263	2067	2070	2076	rVB	55704	76965	1.44%	0.199%
24	14.727	2145	2149	2157	rVB	57469	97254	1.82%	0.251%
25	14.886	2172	2176	2183	rVB	206658	214680	4.02%	0.554%
26	15.227	2230	2234	2240	rVB2	49020	70191	1.31%	0.181%
27	15.504	2276	2281	2286	rBV	1051597	1313020	24.58%	3.389%

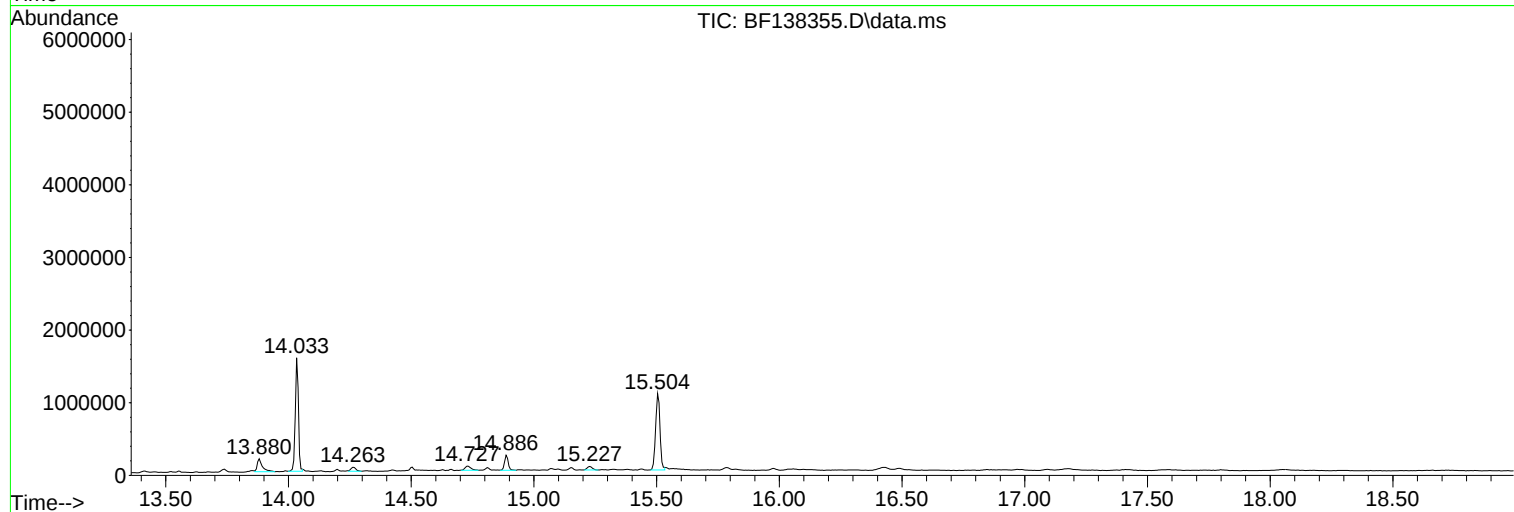
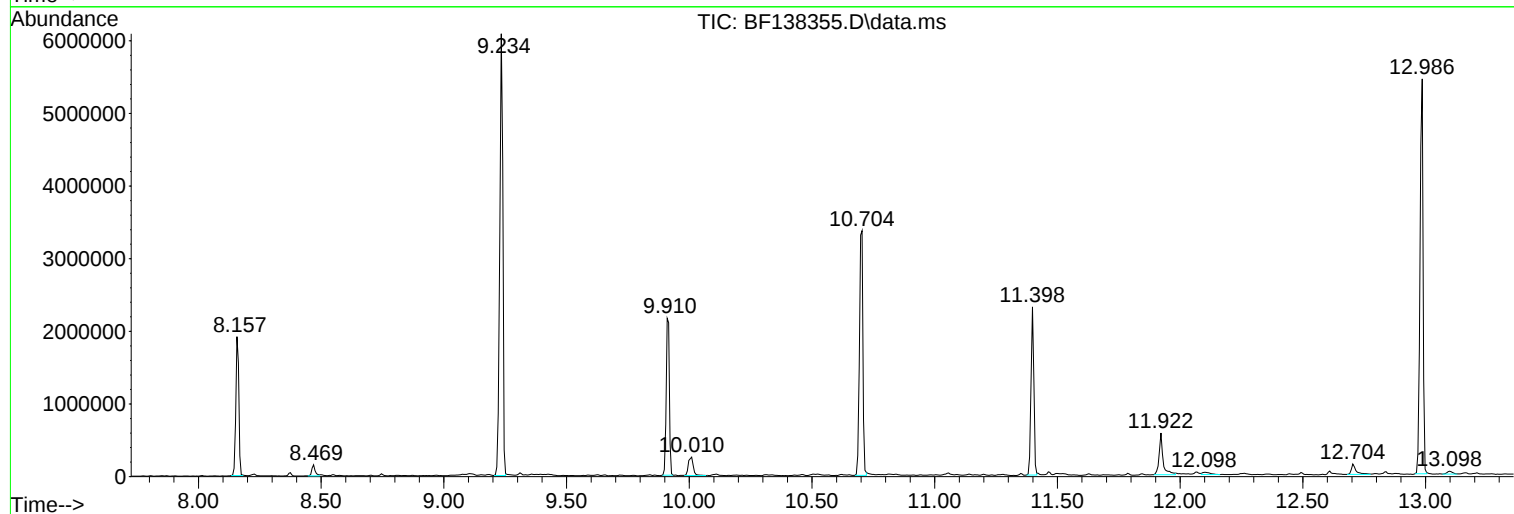
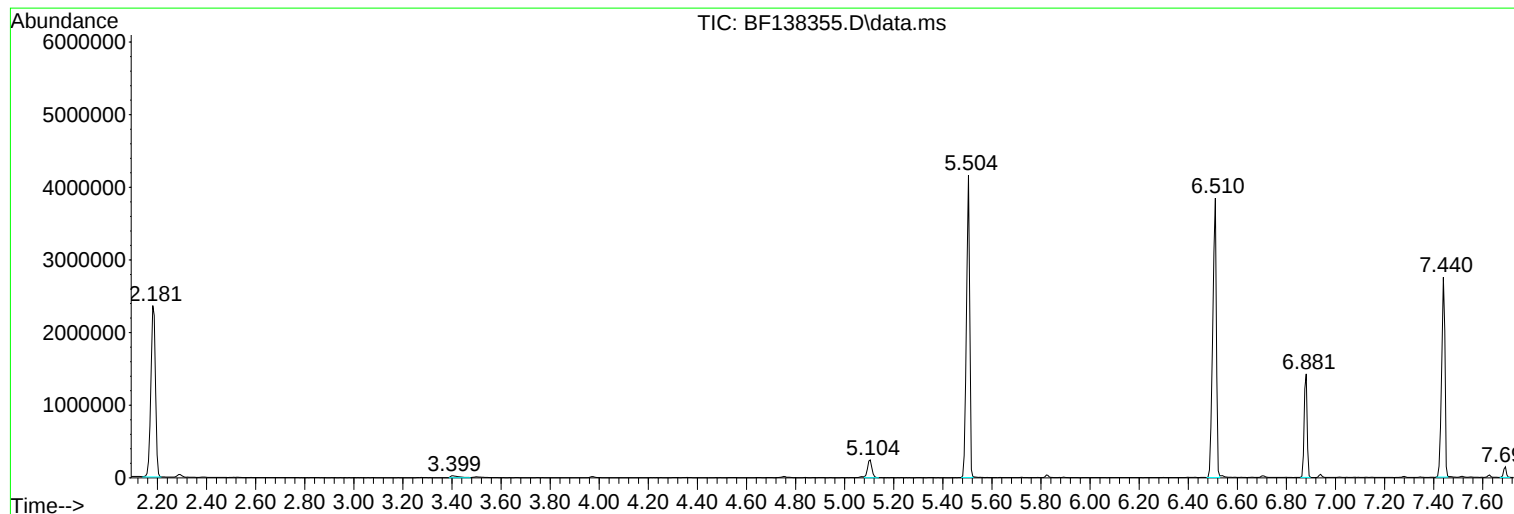
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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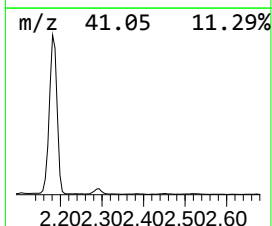
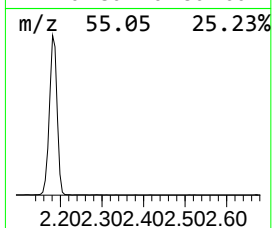
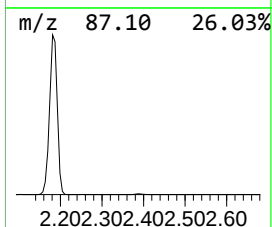
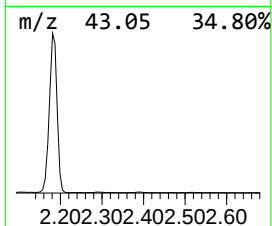
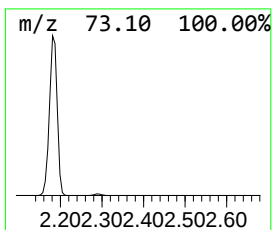
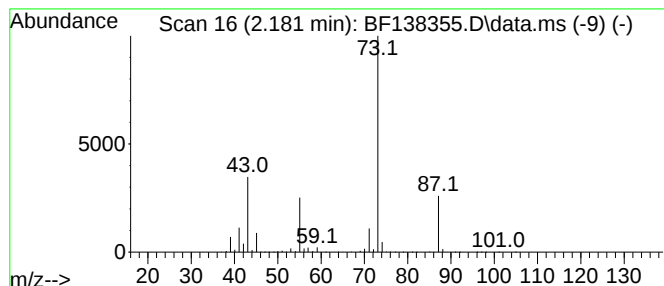
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	50.99 ng	3046840	1,4-Dichlorobenzene-d4	6.881

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



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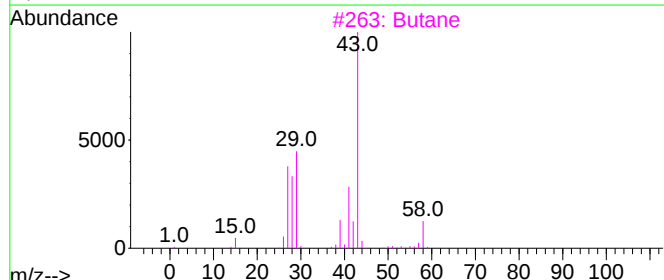
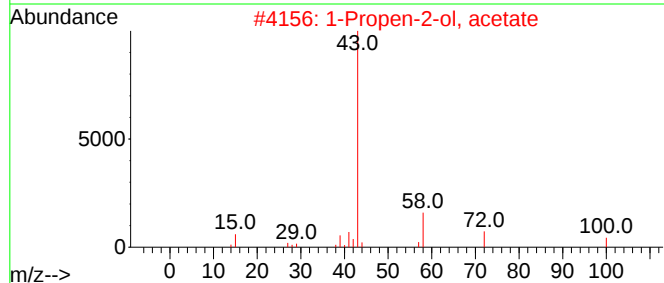
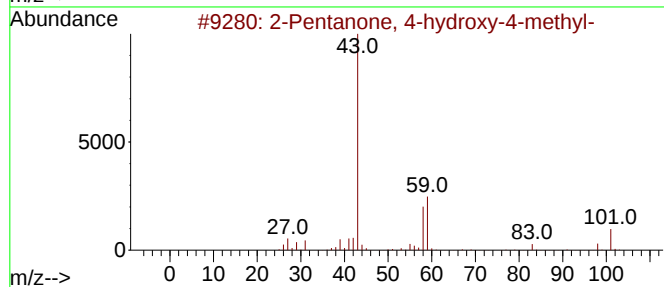
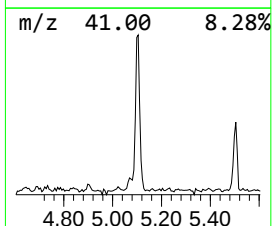
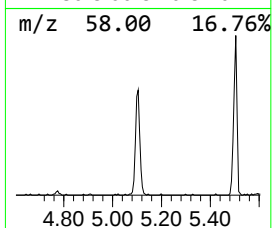
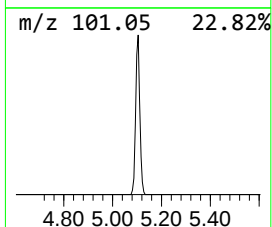
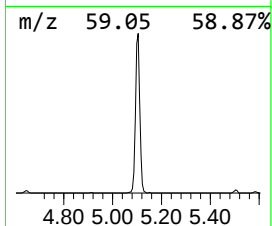
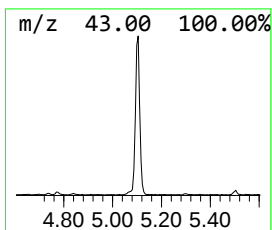
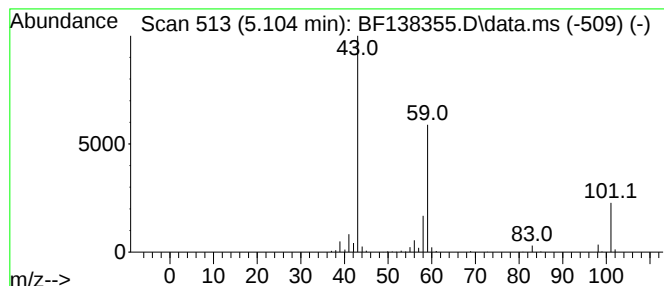
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	5.00 ng	298962	1,4-Dichlorobenzene-d4	6.881

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		Butane	58	C4H10	000106-97-8	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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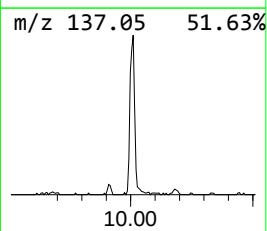
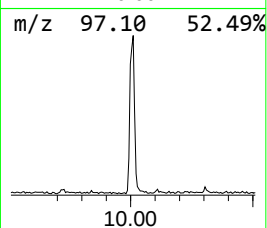
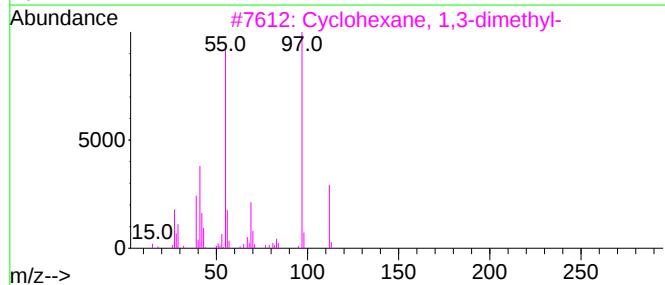
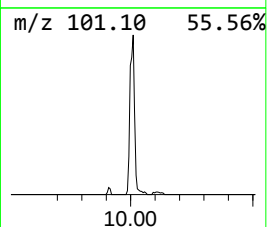
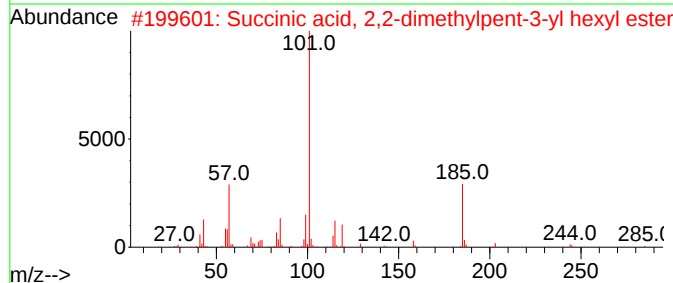
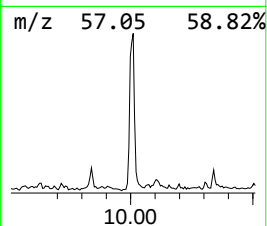
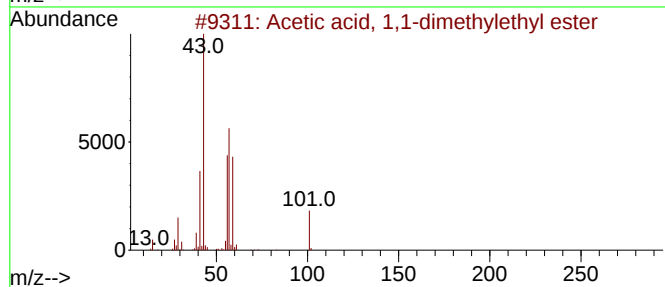
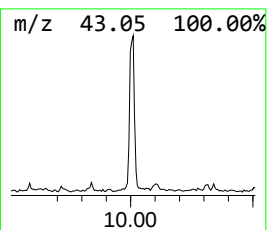
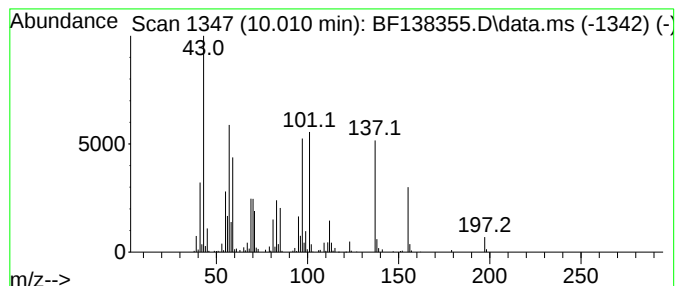
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BNA_F
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown10.010 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.010	3.57 ng	345981	Acenaphthene-d10	9.916	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	22
2	Succinic acid, 2,2-dimethylpent-...	300	C17H32O4	1000381-73-4	14
3	Cyclohexane, 1,3-dimethyl-	112	C8H16	000591-21-9	11
4	Acetaldehyde, 2-butenylhydrazone	112	C6H12N2	075268-07-4	11
5	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	11



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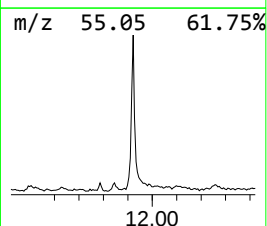
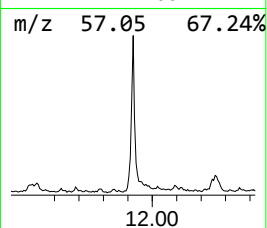
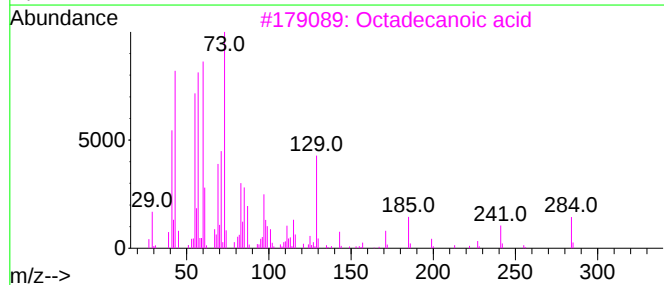
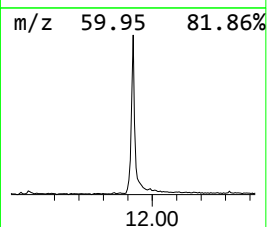
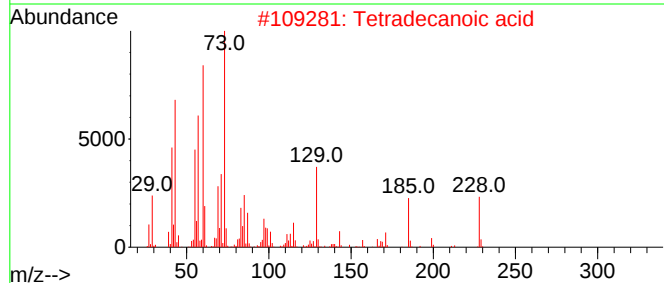
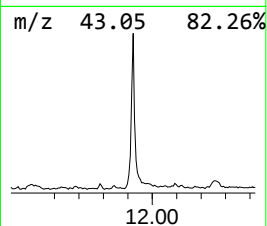
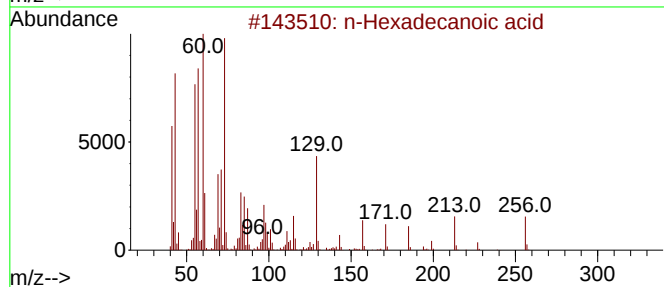
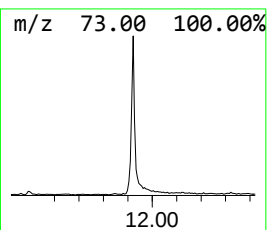
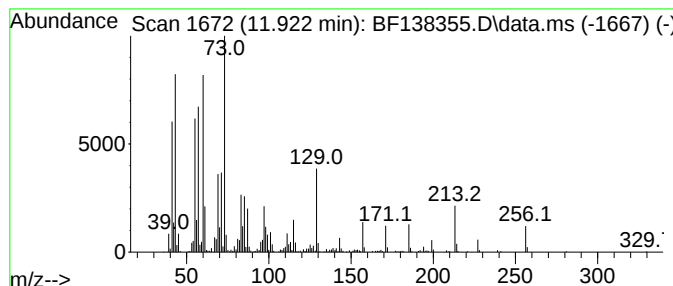
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	6.86 ng	640182	Phenanthrene-d10	11.398

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	94
3			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Tridecanoic acid	214	C13H26O2	000638-53-9	91
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	87



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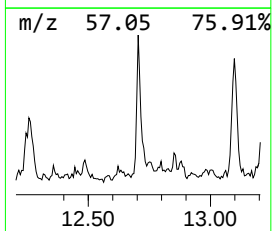
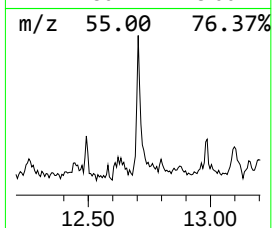
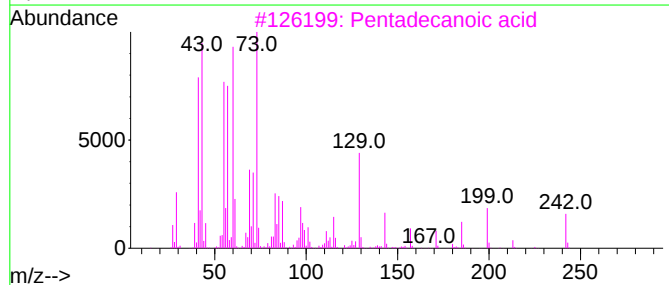
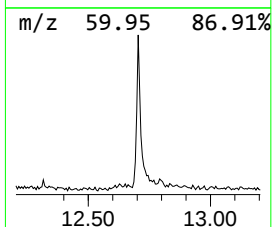
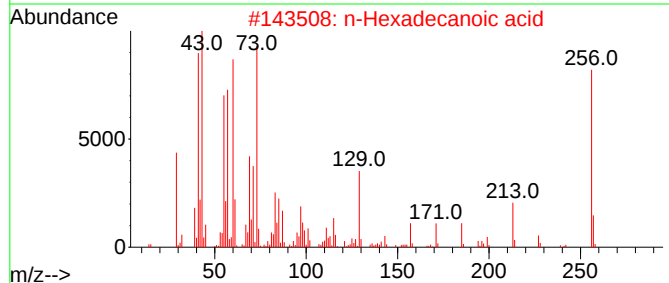
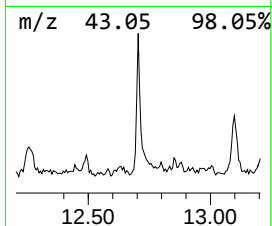
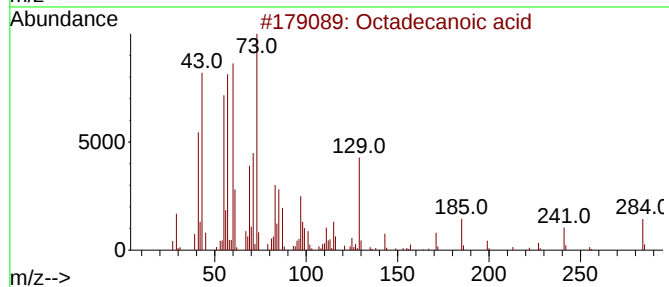
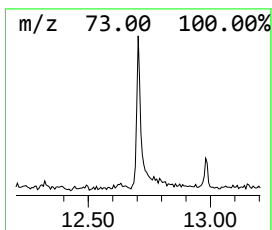
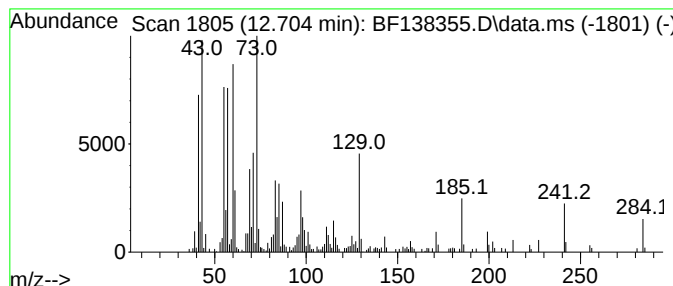
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	2.03 ng	188944	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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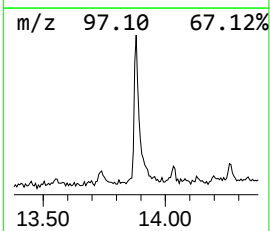
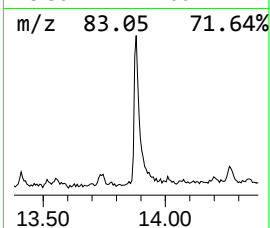
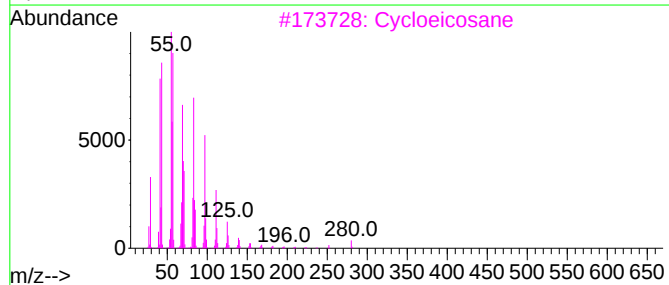
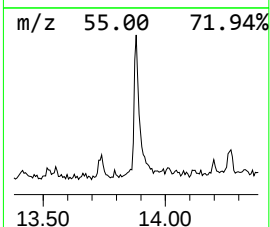
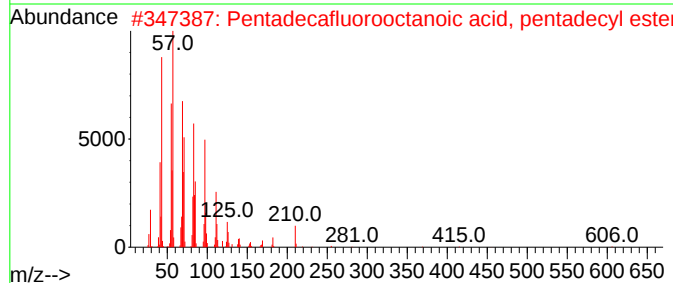
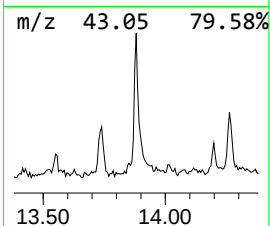
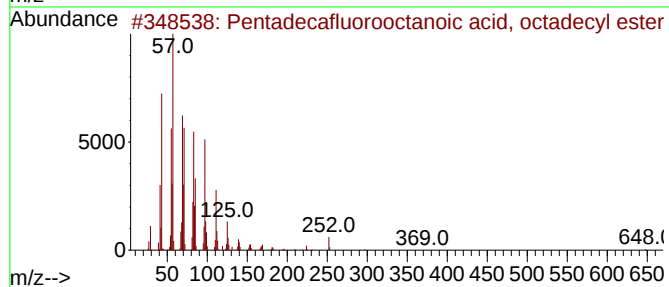
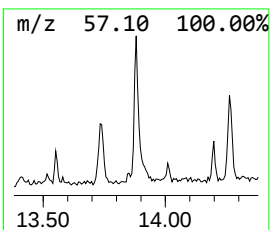
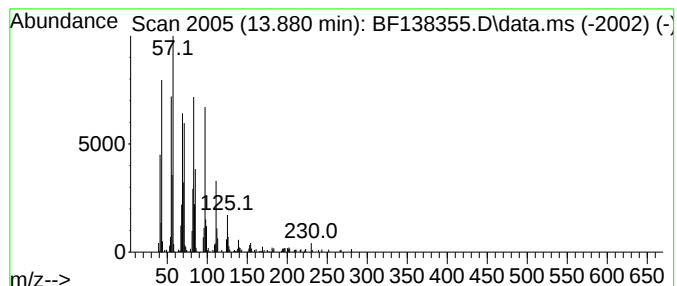
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	3.66 ng	254820	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	94
3			Cycloeicosane	280	C20H40	000296-56-0	93
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
5			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062624\
Data File : BF138355.D
Acq On : 26 Jun 2024 16:56
Operator : CG\JU
Sample : P2915-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-NORTH-1

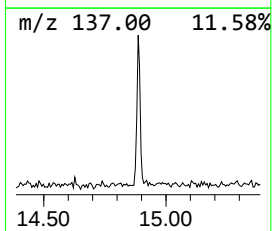
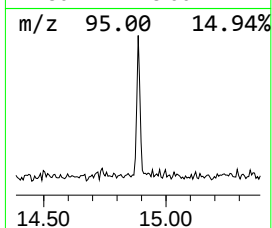
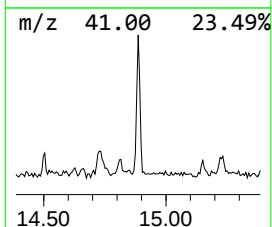
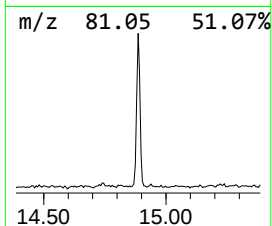
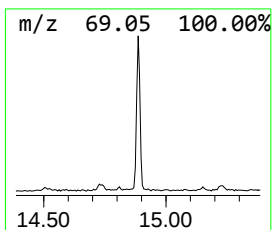
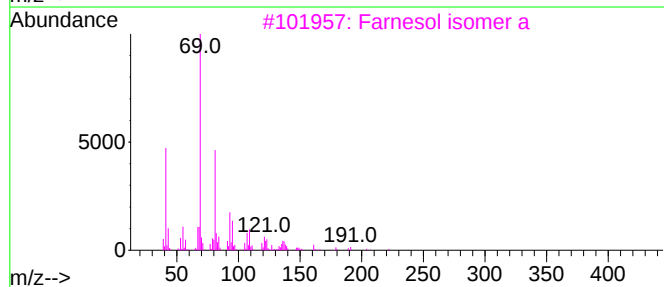
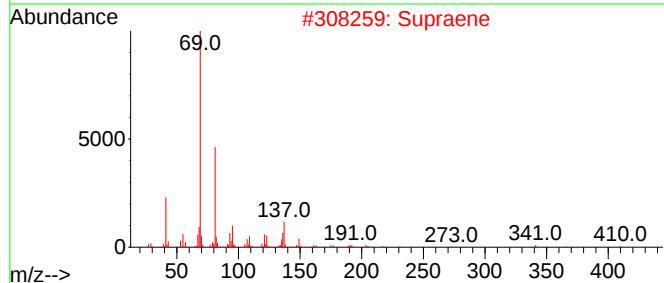
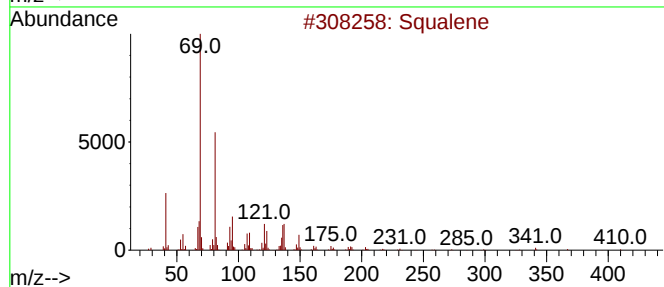
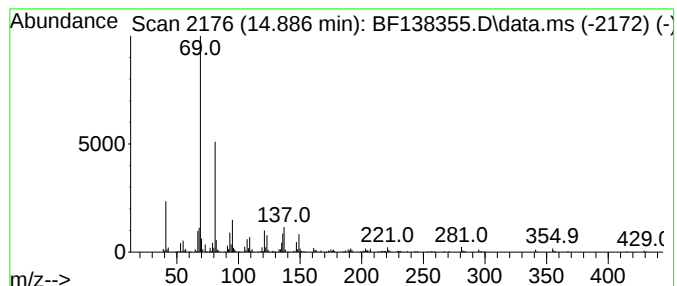
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.886	3.27 ng	214680	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	90
2			Supraene	410	C30H50	007683-64-9	83
3			Farnesol isomer a	222	C15H26O	1000108-92-4	81
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5			3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062624\
Data File : BF138355.D
Acq On : 26 Jun 2024 16:56
Operator : CG\JU
Sample : P2915-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-NORTH-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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...	2.181	51.0	ng	3046840	1	6.881	1195100	20.0
2-Pentanone, 4-...	5.104	5.0	ng	298962	1	6.881	1195100	20.0
unknown10.010	10.010	3.6	ng	345981	3	9.916	1938490	20.0
n-Hexadecanoic ...	11.922	6.9	ng	640182	4	11.398	1865730	20.0
Octadecanoic acid	12.704	2.0	ng	188944	4	11.398	1865730	20.0
Pentadecafluoro...	13.880	3.7	ng	254820	5	14.033	1391860	20.0
Squalene	14.886	3.3	ng	214680	6	15.504	1313020	20.0