

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
 Data File : BF132666.D
 Acq On : 07 Mar 2023 00:25
 Operator : CG\JU
 Sample : 01820-03 2X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HR-4-03032023

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-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132666.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.216	444	447	455	rVB	693952	706206	8.16%	1.453%
2	5.616	512	515	527	rVB	1654325	1518731	17.56%	3.125%
3	6.616	681	685	694	rBV	1723939	1481643	17.13%	3.049%
4	6.998	746	750	753	rBV	1385650	1120460	12.95%	2.306%
5	7.557	841	845	848	rBV	1202141	957689	11.07%	1.971%
6	8.281	965	968	972	rBV	1457666	1338120	15.47%	2.753%
7	9.357	1147	1151	1154	rBV	2040034	1628103	18.82%	3.350%
8	9.616	1192	1195	1200	rBV2	161704	133968	1.55%	0.276%
9	10.045	1264	1268	1271	rBV	1567445	1239453	14.33%	2.550%
10	10.757	1385	1389	1392	rVB	350084	266612	3.08%	0.549%
11	10.834	1399	1402	1411	rBV	840379	743381	8.59%	1.530%
12	10.934	1416	1419	1426	rBV2	73179	103272	1.19%	0.213%
13	11.539	1518	1522	1525	rBV	1355014	1151070	13.31%	2.369%
14	11.563	1525	1526	1530	rVB	150905	101795	1.18%	0.209%
15	11.922	1582	1587	1590	rBV	3012223	2939435	33.98%	6.049%
16	12.057	1606	1610	1619	rBV	734953	802349	9.28%	1.651%
17	12.304	1649	1652	1661	rBV4	327493	345923	4.00%	0.712%
18	12.616	1699	1705	1707	rBV	6896773	8649343	100.00%	17.798%
19	12.639	1707	1709	1715	rVV2	7357261	6748302	78.02%	13.886%
20	12.716	1719	1722	1725	rVB	2617484	2102891	24.31%	4.327%
21	12.757	1725	1729	1731	rBV2	1394614	1720097	19.89%	3.539%
22	12.775	1731	1732	1742	rVV2	1308808	1155070	13.35%	2.377%
23	12.845	1742	1744	1750	rVB3	258070	288481	3.34%	0.594%
24	12.998	1764	1770	1776	rBV	383873	480926	5.56%	0.990%
25	13.133	1789	1793	1796	rBV	1566668	1314130	15.19%	2.704%
26	13.445	1843	1846	1848	rBV2	264277	212644	2.46%	0.438%
27	13.475	1848	1851	1856	rVV7	110213	160196	1.85%	0.330%
28	13.516	1856	1858	1862	rVV3	128507	160817	1.86%	0.331%
29	13.874	1916	1919	1923	rBV2	239022	318457	3.68%	0.655%
30	14.116	1958	1960	1963	rBV	289966	267284	3.09%	0.550%
31	14.204	1970	1975	1978	rBV2	1260970	1393792	16.11%	2.868%
32	15.504	2193	2196	2204	rVB	332658	521349	6.03%	1.073%
33	15.763	2236	2240	2244	rVB	682919	895419	10.35%	1.843%
34	16.033	2282	2286	2294	rVB	405537	681281	7.88%	1.402%
35	16.668	2389	2394	2405	rVB2	466244	1065927	12.32%	2.193%
36	17.439	2519	2525	2538	rVB2	607761	1642012	18.98%	3.379%

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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-BF022223.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.386	2678	2686	2704	rVB2	605464	2240647	25.91%	4.611%
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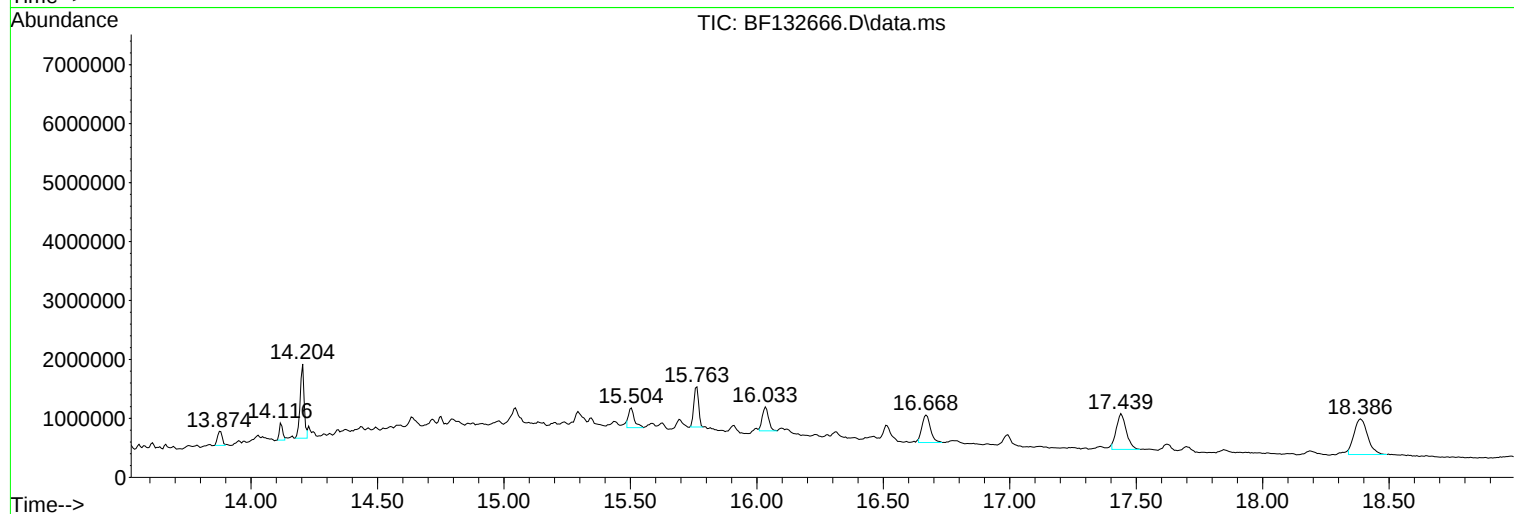
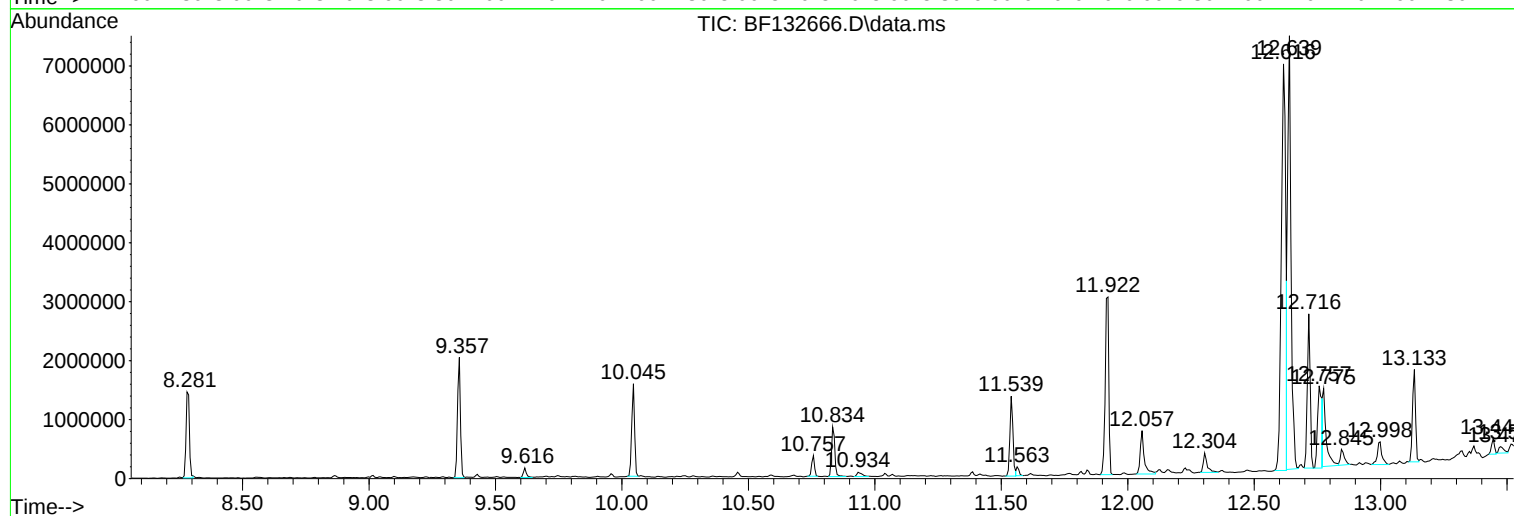
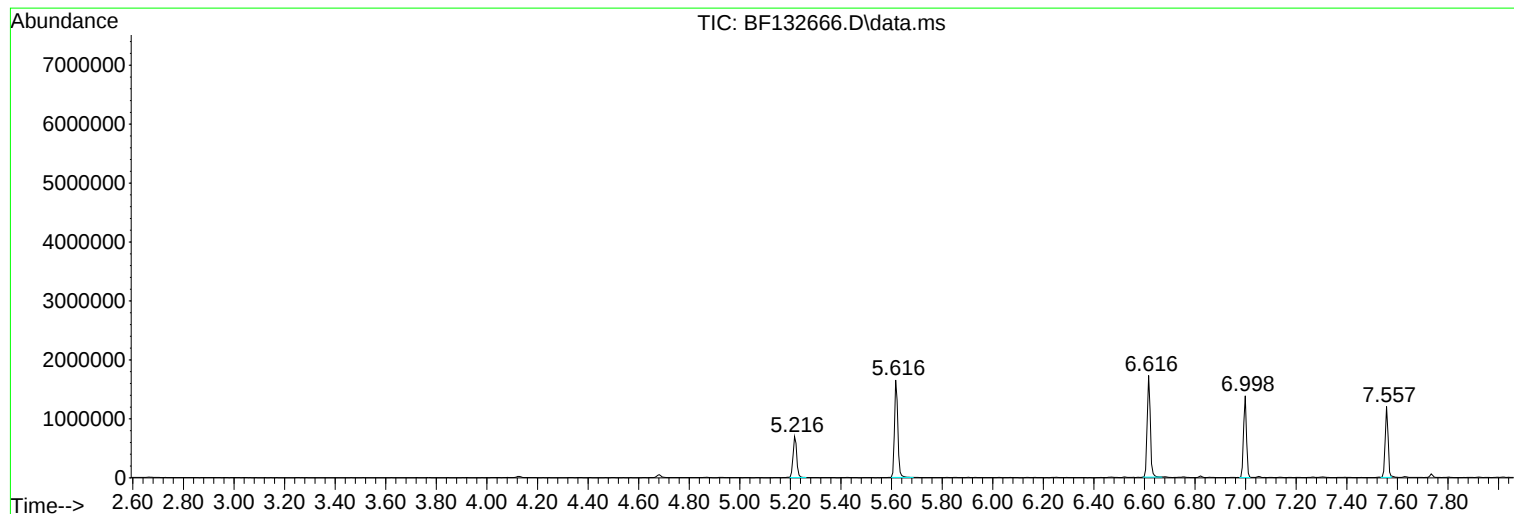
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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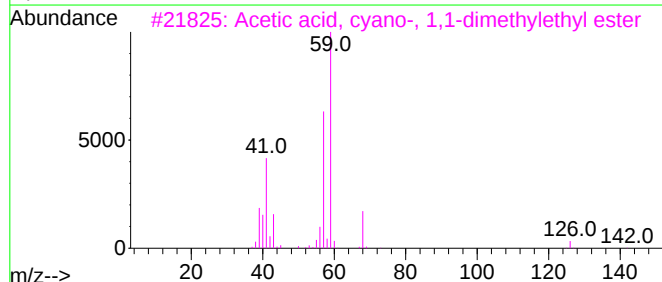
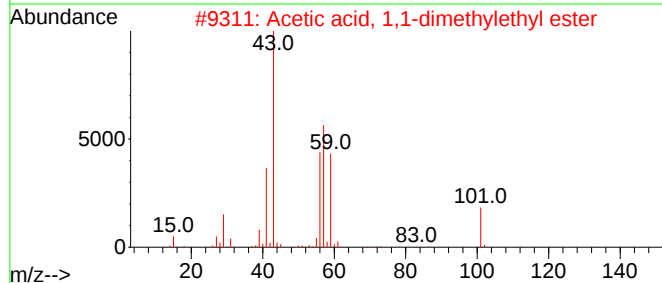
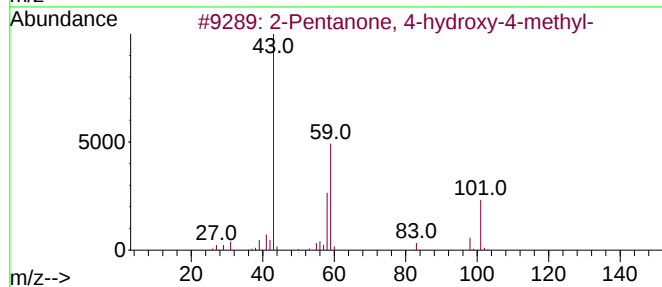
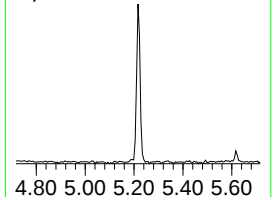
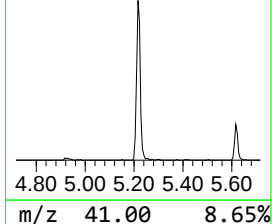
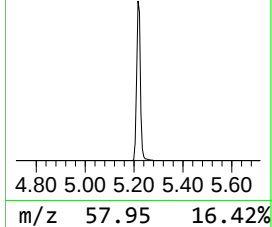
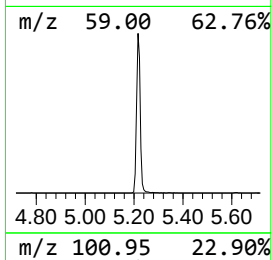
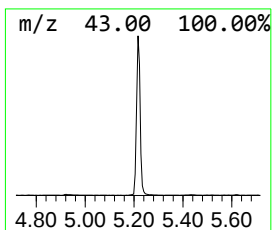
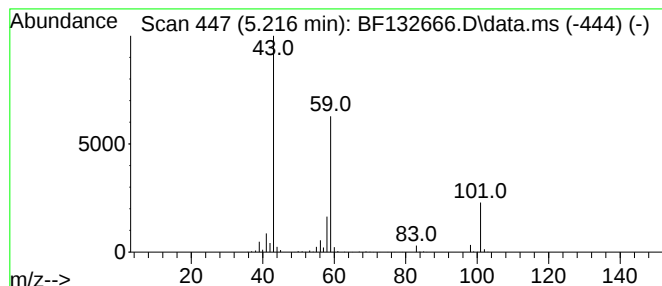
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.216	12.61 ng	706206	1,4-Dichlorobenzene-d4	6.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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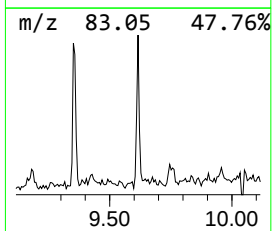
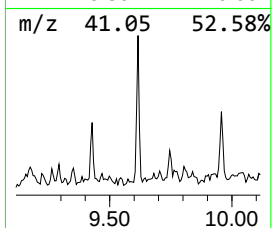
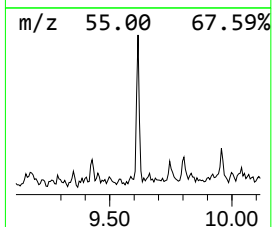
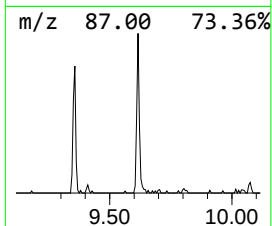
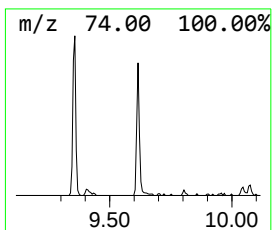
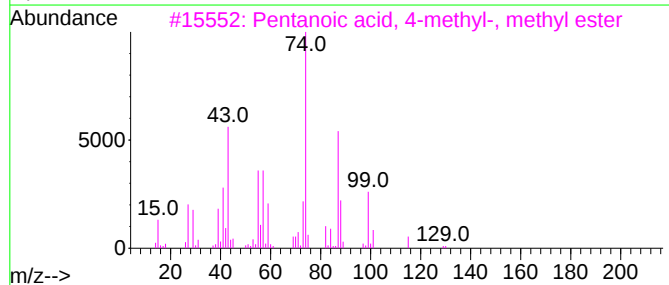
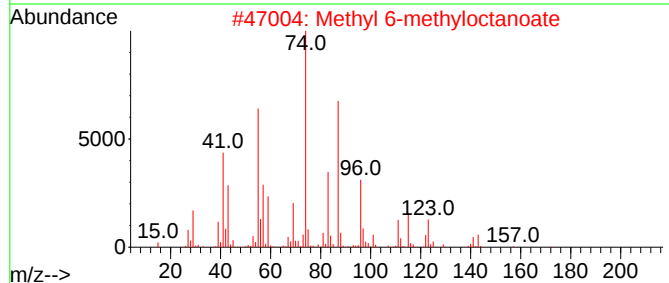
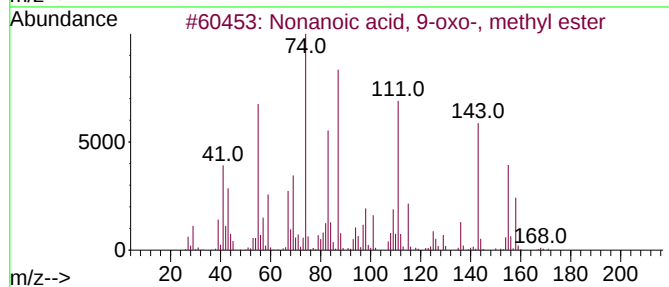
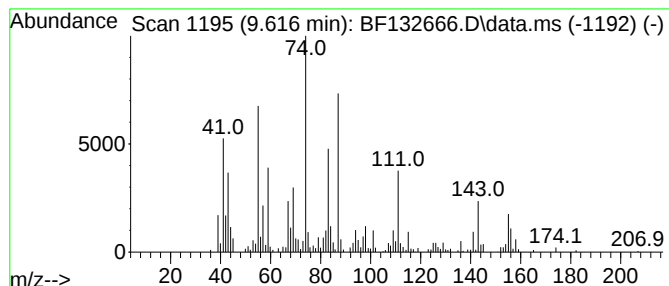
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Nonanoic acid, 9-oxo-, meth... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.616	2.16 ng	133968	Acenaphthene-d10	10.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid, 9-oxo-, methyl ester	186	C10H18O3	001931-63-1	90
2			Methyl 6-methyloctanoate	172	C10H20O2	005129-62-4	59
3			Pentanoic acid, 4-methyl-, methy...	130	C7H14O2	002412-80-8	43
4			Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	35
5			Butanoic acid, 4-chloro-, methyl...	136	C5H9ClO2	003153-37-5	22



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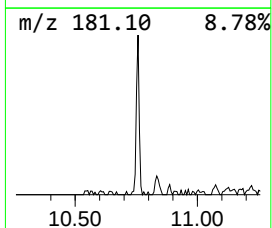
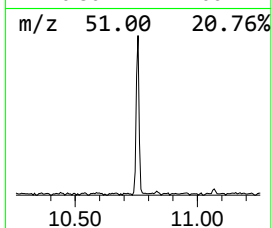
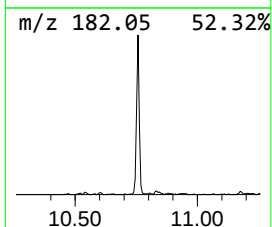
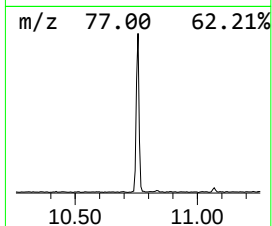
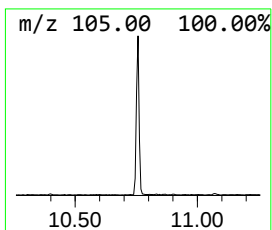
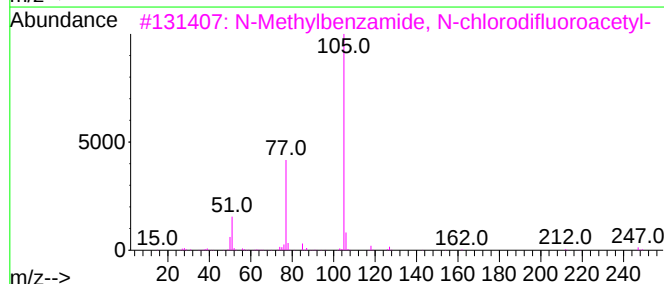
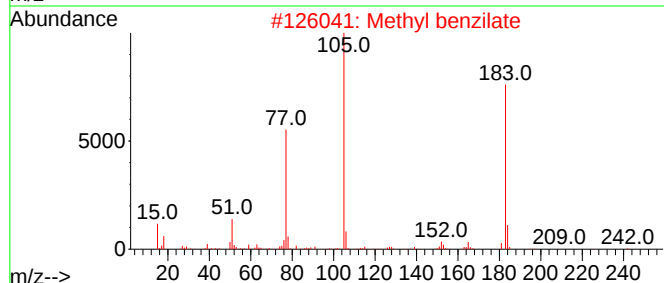
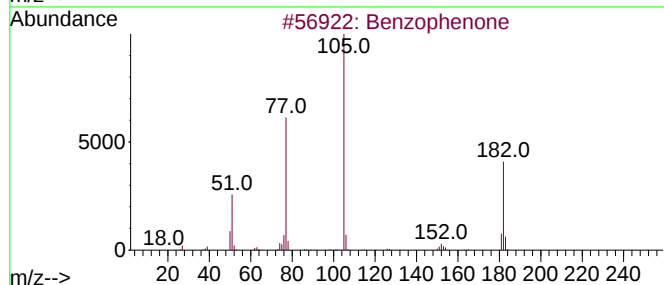
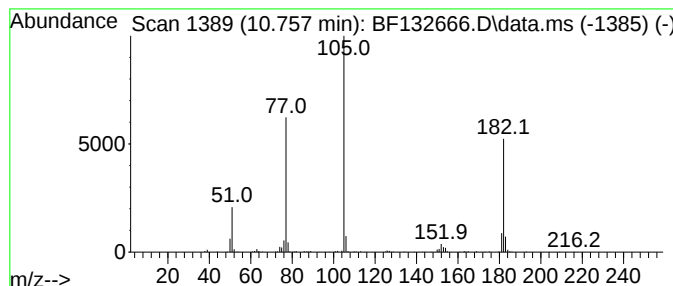
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.757	4.30 ng	266612	Acenaphthene-d10	10.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Methyl benzoate	242	C15H14O3	000076-89-1	47
3			N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	47
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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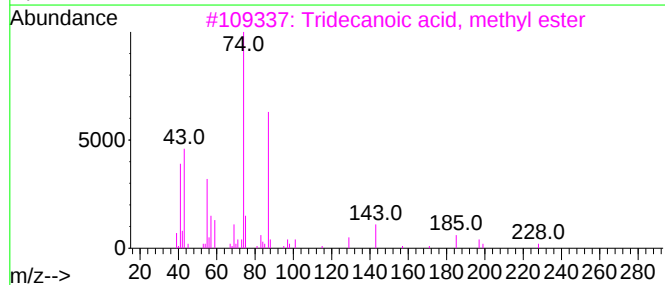
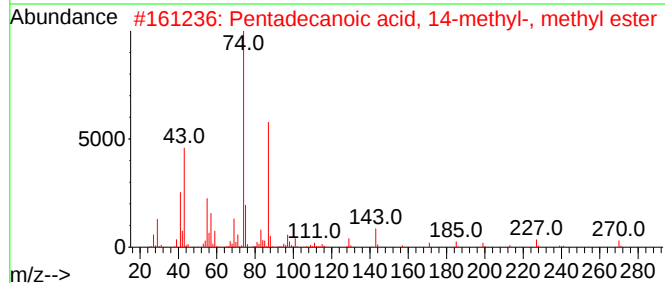
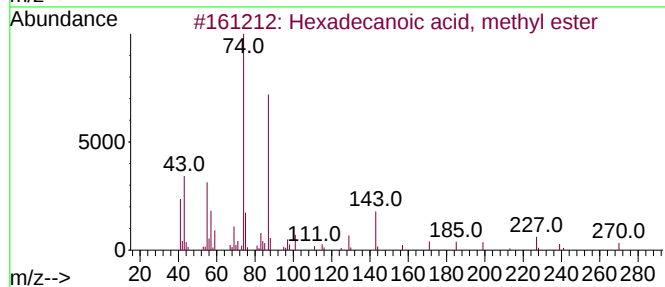
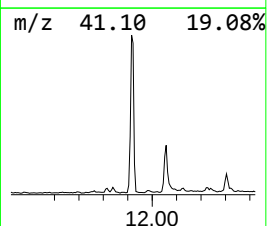
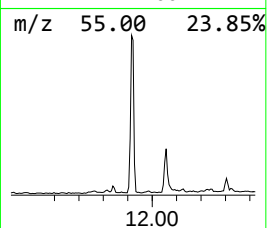
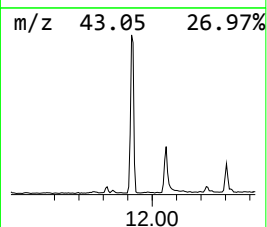
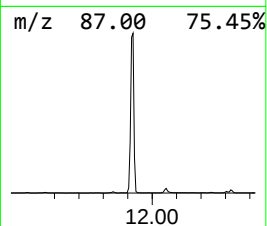
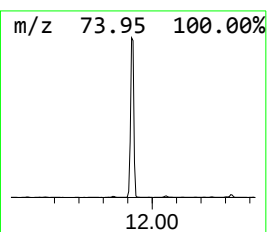
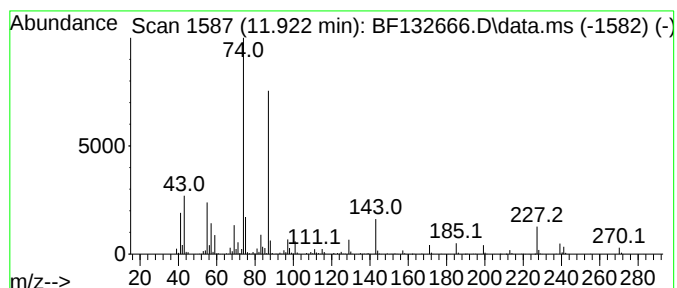
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.922	51.07 ng	2939440	Phenanthrene-d10		11.539	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester		270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...		270	C17H34O2	005129-60-2	96
3	Tridecanoic acid, methyl ester		228	C14H28O2	001731-88-0	91
4	Pentadecanoic acid, methyl ester		256	C16H32O2	007132-64-1	86
5	Decanoic acid, methyl ester		186	C11H22O2	000110-42-9	83



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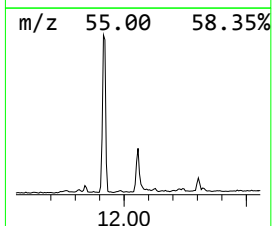
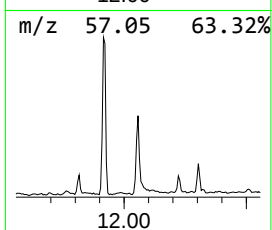
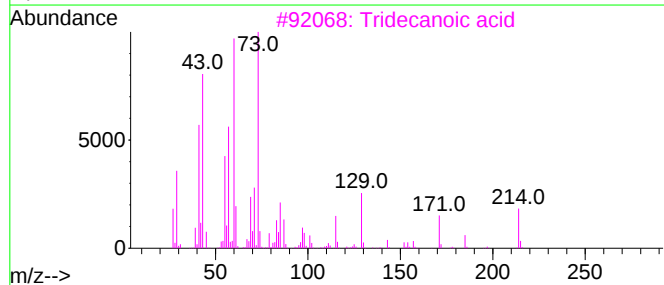
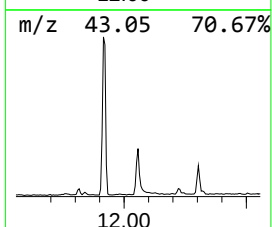
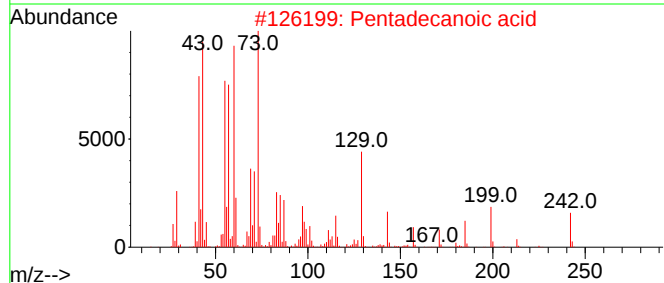
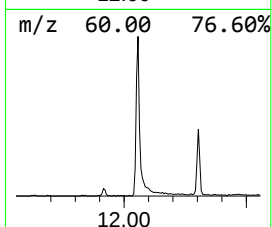
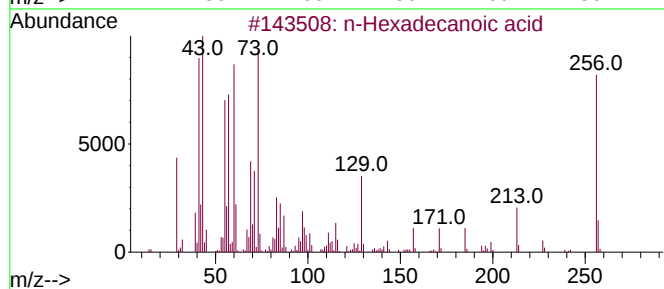
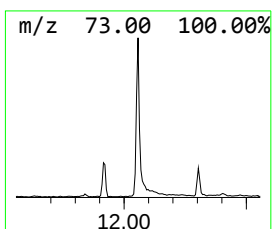
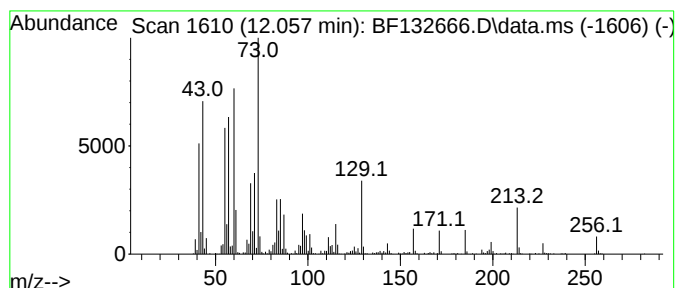
Instrument :
BNA_F
ClientSampleId :
HR-4-03032023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.057	13.94 ng	802349	Phenanthrene-d10	11.539	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
Data File : BF132666.D
Acq On : 07 Mar 2023 00:25
Operator : CG\JU
Sample : 01820-03 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HR-4-03032023

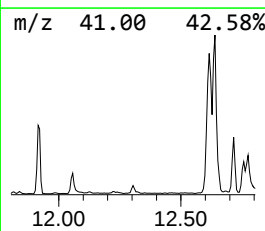
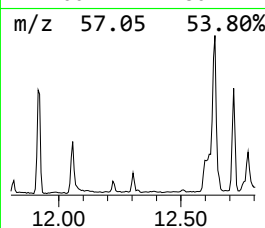
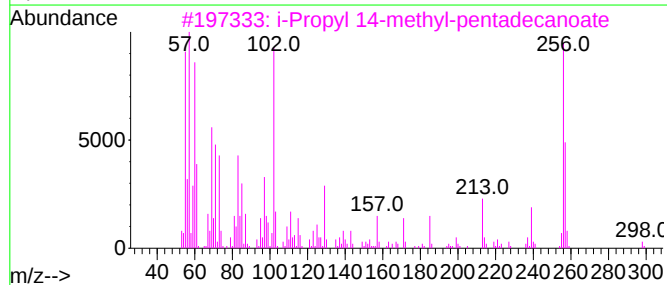
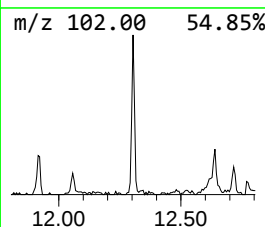
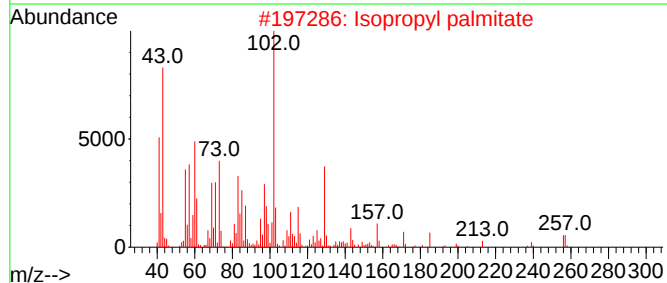
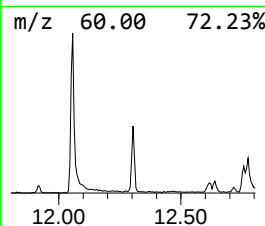
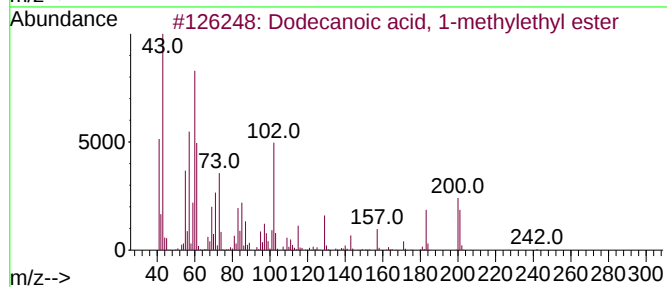
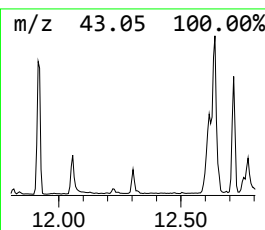
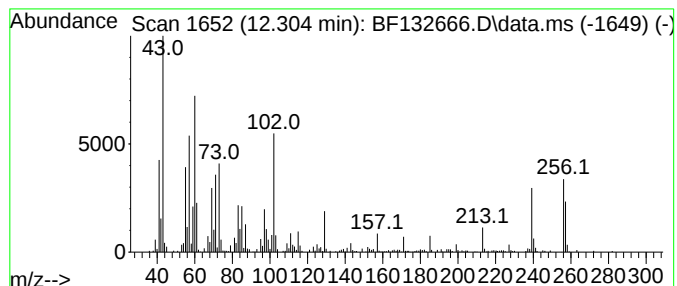
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dodecanoic acid, 1-methylet... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.304	6.01 ng	345923	Phenanthrene-d10	11.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	89
2			Isopropyl palmitate	298	C19H38O2	000142-91-6	87
3			i-Propyl 14-methyl-pentadecanoate	298	C19H38O2	1000336-62-4	52
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
5			8-Methylnonanoic acid, isopropyl...	214	C13H26O2	1000452-00-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
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Sample : 01820-03 2X
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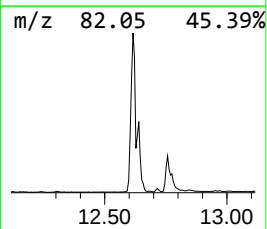
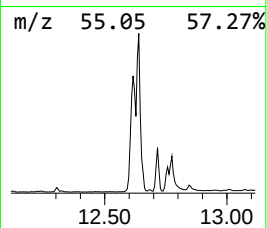
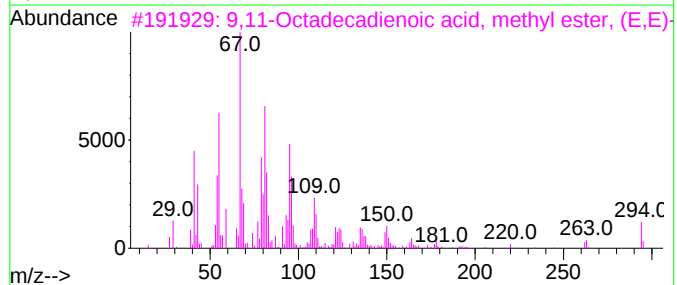
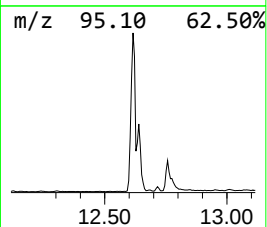
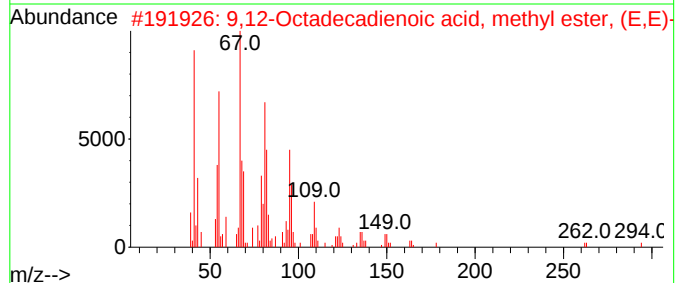
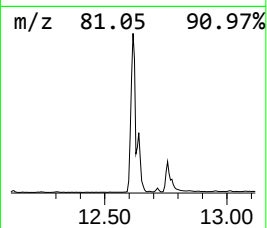
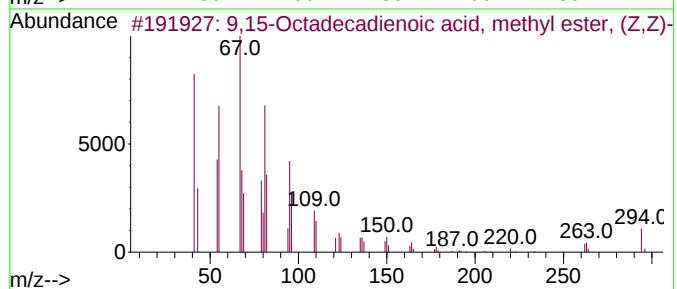
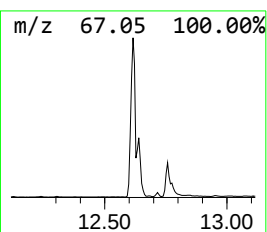
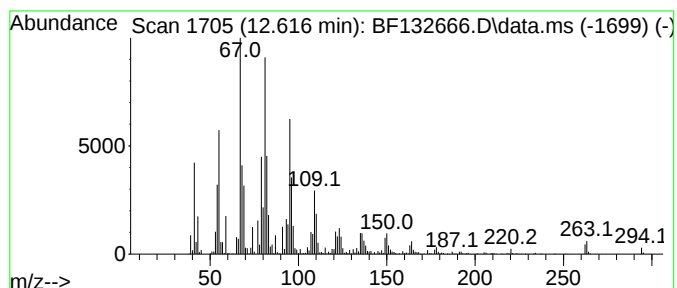
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9,15-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.616	150.28 ng	8649340	Phenanthrene-d10	11.539	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
3	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	97
4	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	96
5	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
Data File : BF132666.D
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Operator : CG\JU
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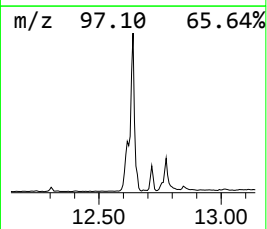
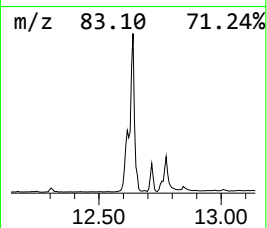
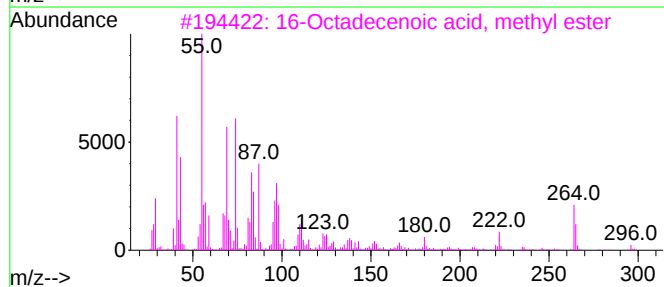
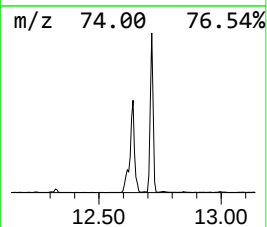
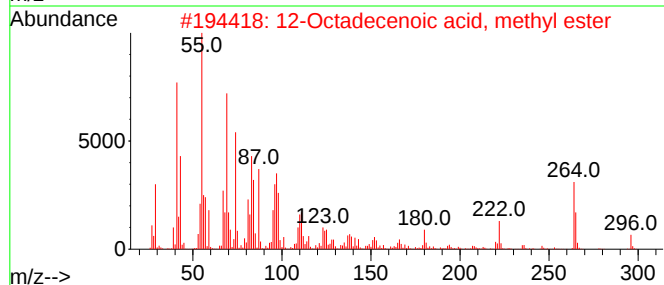
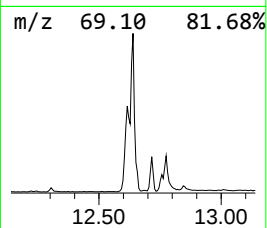
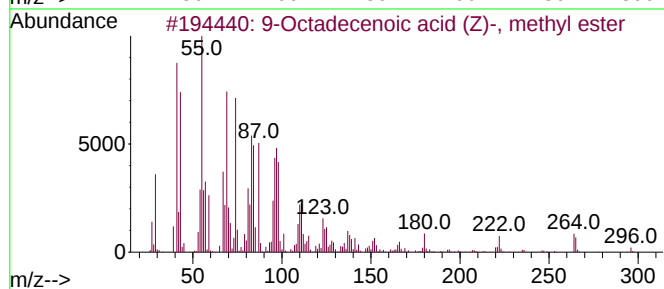
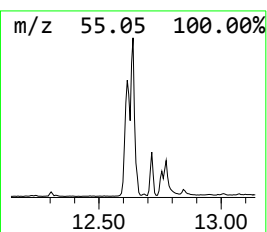
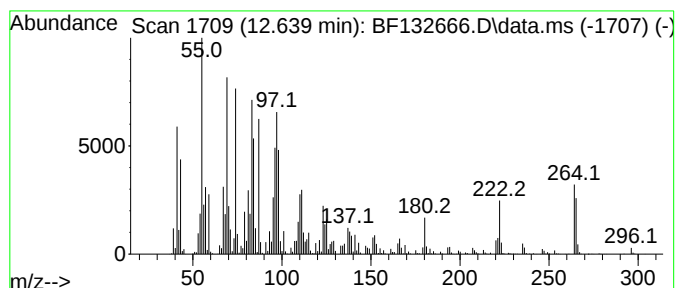
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HR-4-03032023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.639	117.25 ng	6748300	Phenanthrene-d10	11.539	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
4	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
Data File : BF132666.D
Acq On : 07 Mar 2023 00:25
Operator : CG\JU
Sample : 01820-03 2X
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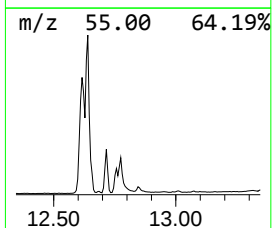
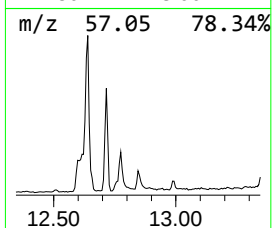
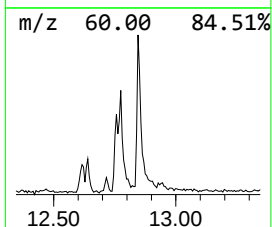
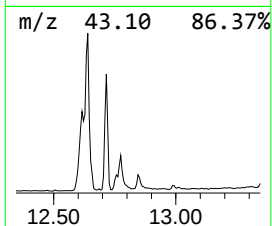
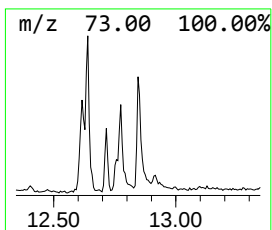
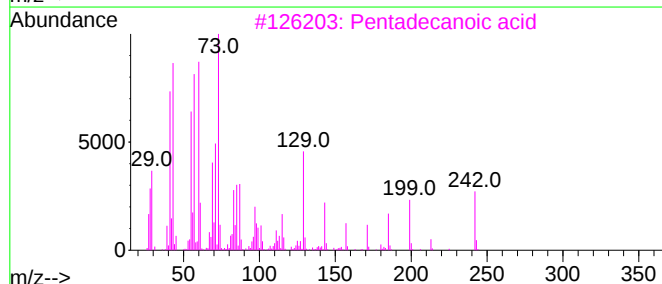
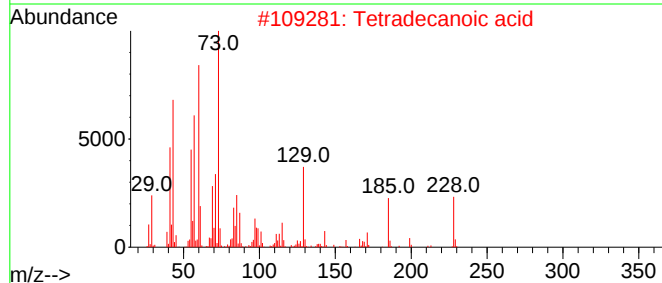
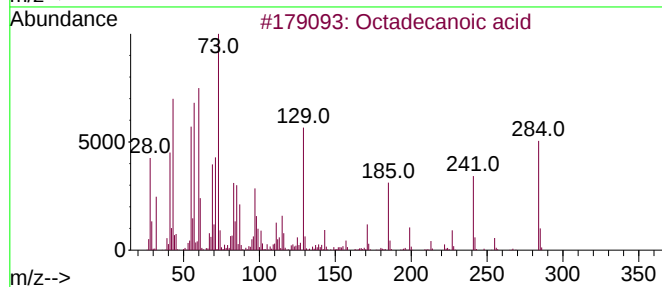
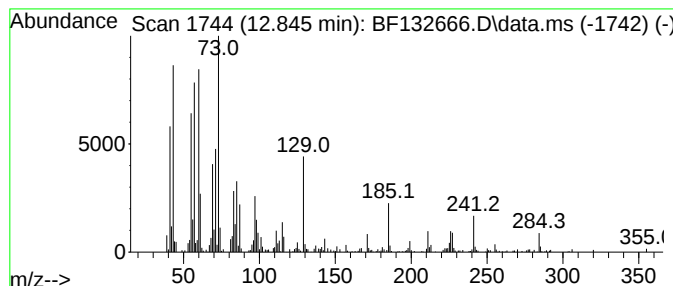
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.845	5.01 ng	288481	Phenanthrene-d10	11.539	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
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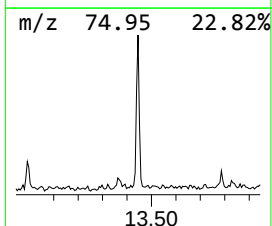
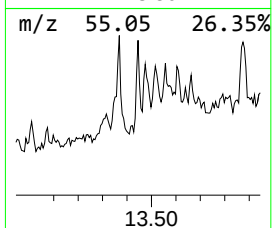
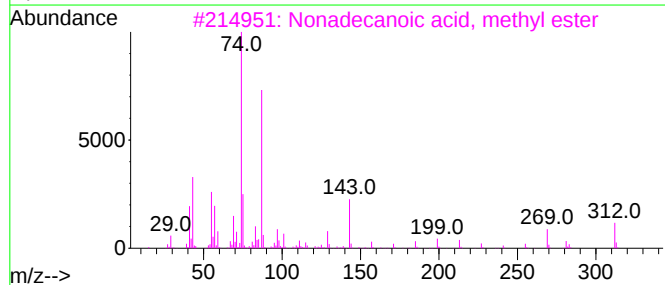
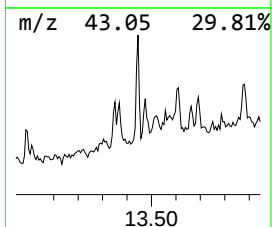
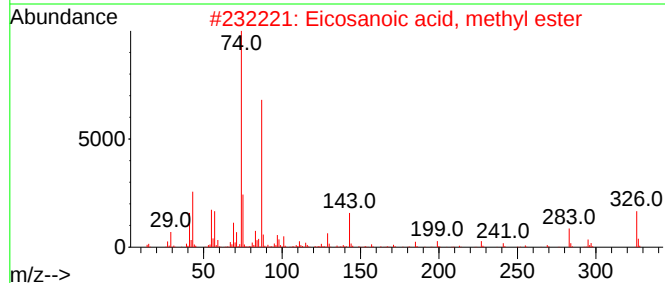
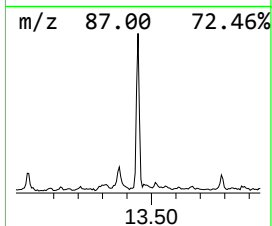
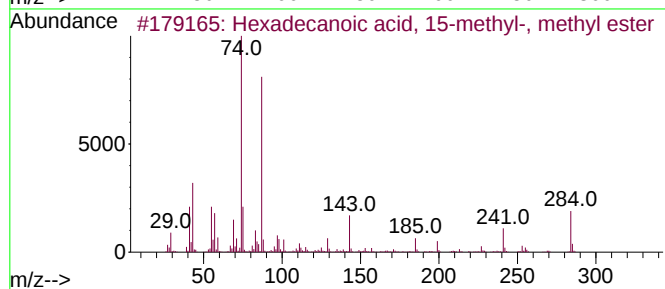
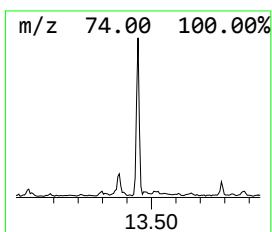
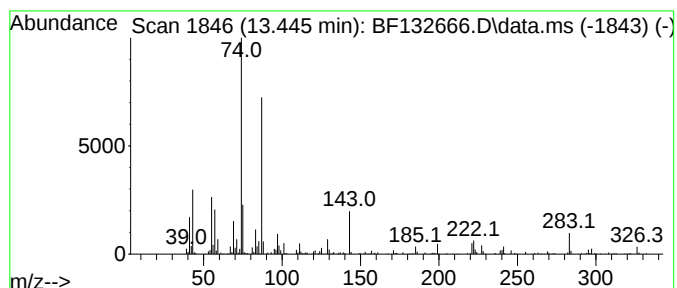
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecanoic acid, 15-methy... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.445	3.05 ng	212644	Chrysene-d12		14.204	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 15-methyl-, m...		284	C18H36O2	006929-04-0	95
2	Eicosanoic acid, methyl ester		326	C21H42O2	001120-28-1	91
3	Nonadecanoic acid, methyl ester		312	C20H40O2	001731-94-8	87
4	Methyl stearate		298	C19H38O2	000112-61-8	83
5	Heptadecanoic acid, methyl ester		284	C18H36O2	001731-92-6	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
Data File : BF132666.D
Acq On : 07 Mar 2023 00:25
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ALS Vial : 19 Sample Multiplier: 1

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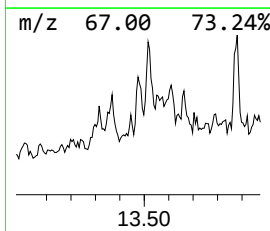
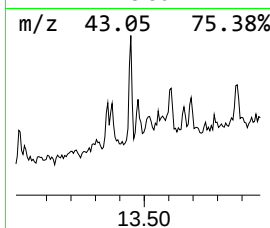
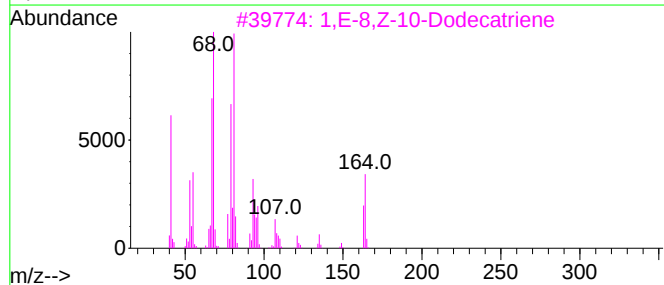
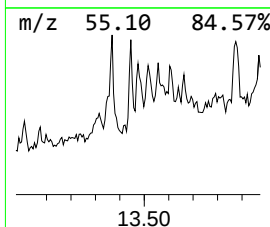
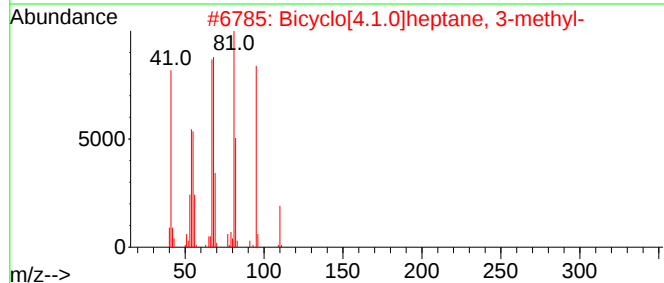
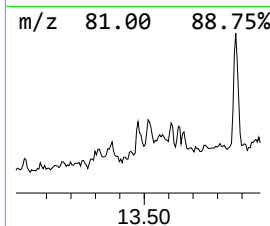
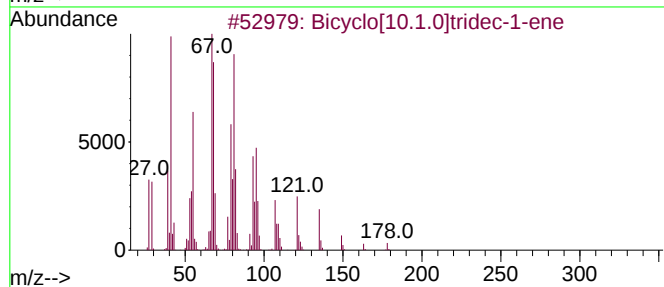
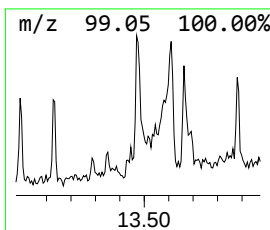
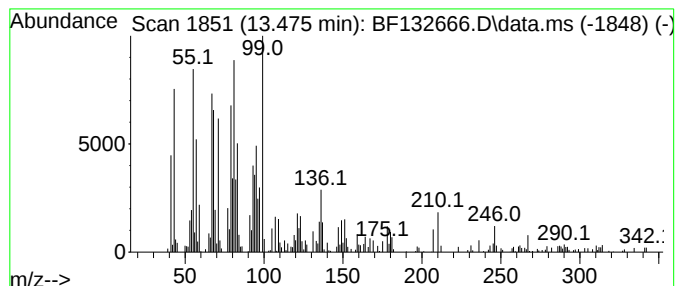
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown13.475 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.475	2.30 ng	160196	Chrysene-d12	14.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[10.1.0]tridec-1-ene	178	C13H22	054766-91-5	46
2			Bicyclo[4.1.0]heptane, 3-methyl-	110	C8H14	041977-47-3	43
3			1,E-8,Z-10-Dodecatriene	164	C12H20	1000098-05-5	42
4			8,10-Dodecadien-1-ol, acetate, (...	224	C14H24O2	053880-51-6	35
5			Fumaric acid, 4-octyl hex-4-yn-3...	308	C18H28O4	1000405-62-1	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
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Misc :
ALS Vial : 19 Sample Multiplier: 1

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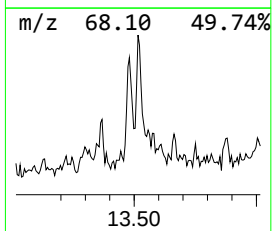
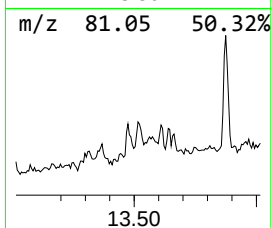
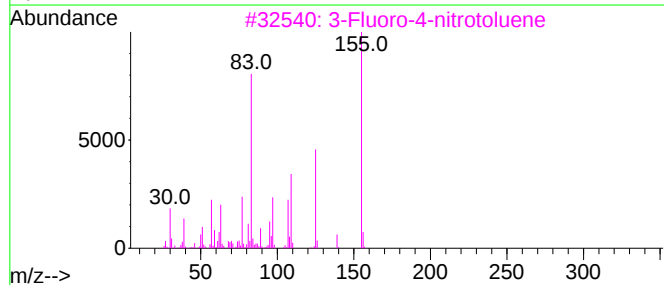
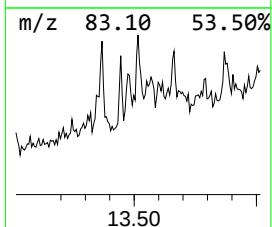
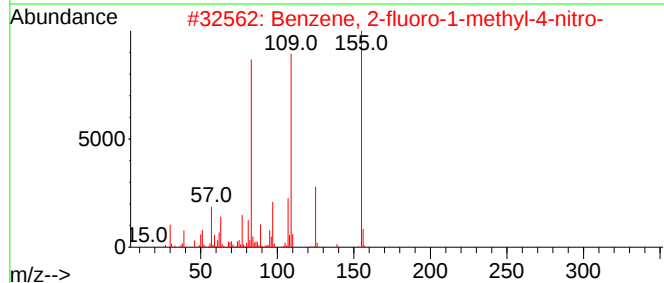
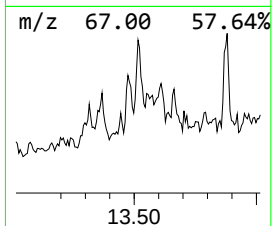
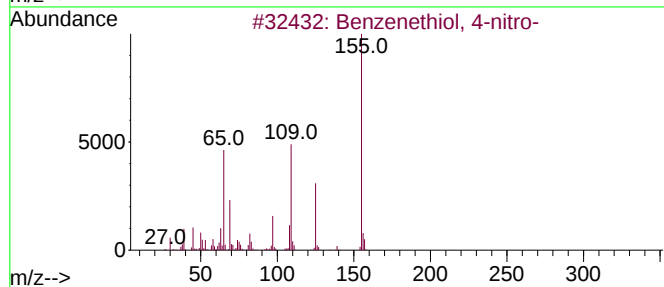
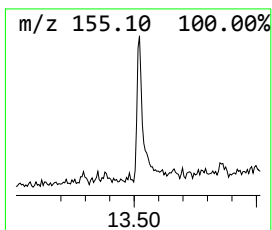
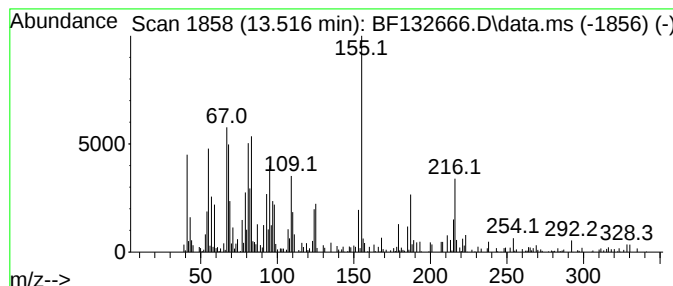
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown13.516 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.516	2.31 ng	160817	Chrysene-d12	14.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenethiol, 4-nitro-	155	C6H5NO2S	001849-36-1	35
2			Benzene, 2-fluoro-1-methyl-4-nitro-	155	C7H6FN02	001427-07-2	27
3			3-Fluoro-4-nitrotoluene	155	C7H6FN02	000446-34-4	25
4			1,2-Cyclohexanedicarboxylic acid...	318	C19H26O4	1000339-82-9	22
5			1,2-Cyclohexanedicarboxylic acid...	352	C21H36O4	1000339-74-2	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
Data File : BF132666.D
Acq On : 07 Mar 2023 00:25
Operator : CG\JU
Sample : 01820-03 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HR-4-03032023

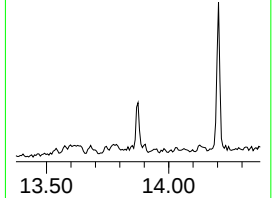
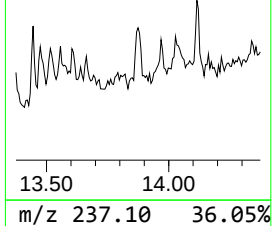
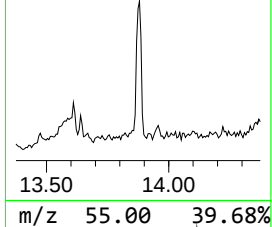
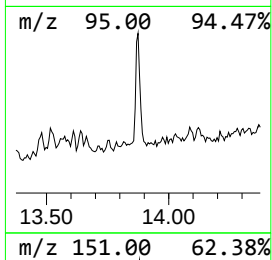
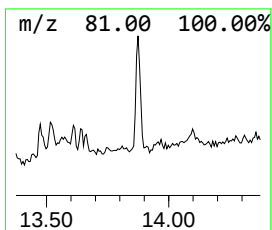
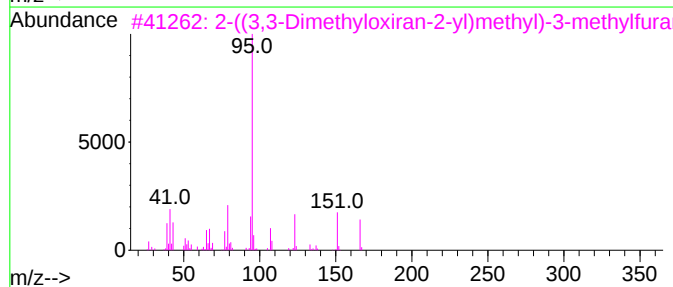
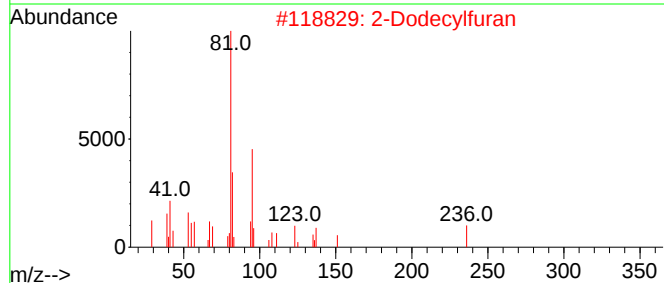
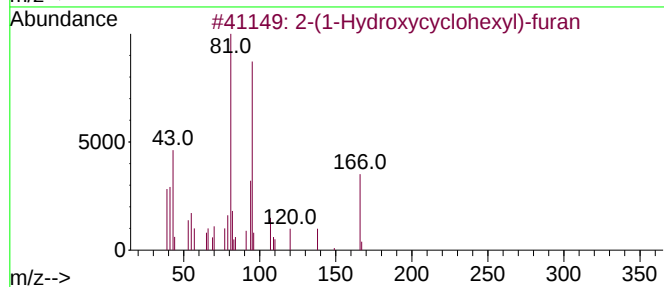
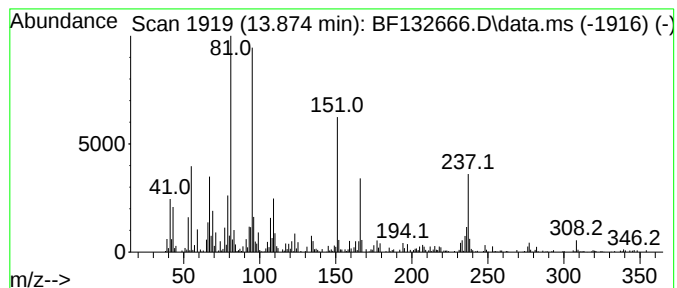
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2-(1-Hydroxycyclohexyl)-furan Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	4.57 ng	318457	Chrysene-d12	14.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-(1-Hydroxycyclohexyl)-furan	166	C10H14O2	036169-67-2	58
2			2-Dodecylfuran	236	C16H28O	075308-12-2	41
3			2-((3,3-Dimethyloxiran-2-yl)methyl)-3-methylfuran	166	C10H14O2	092356-06-4	30
4			Bicyclo[2.2.1]heptan-2-one, 1,3-diol	166	C11H18O	005811-48-3	30
5			Tricyclo[4.3.1.1(3,8)]undecan-3-ol	166	C11H18O	014504-80-4	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
Data File : BF132666.D
Acq On : 07 Mar 2023 00:25
Operator : CG\JU
Sample : 01820-03 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

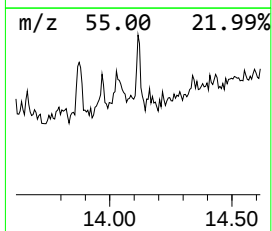
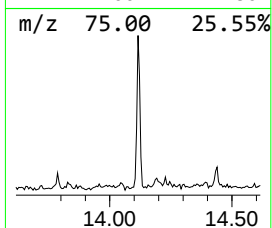
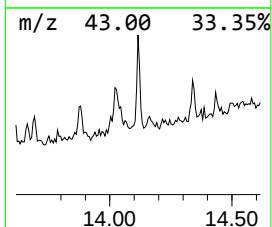
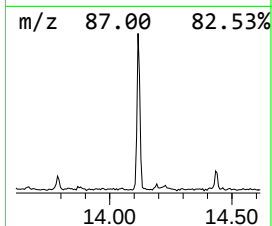
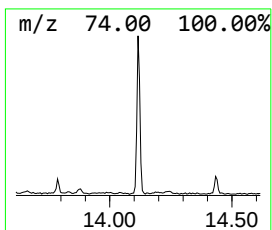
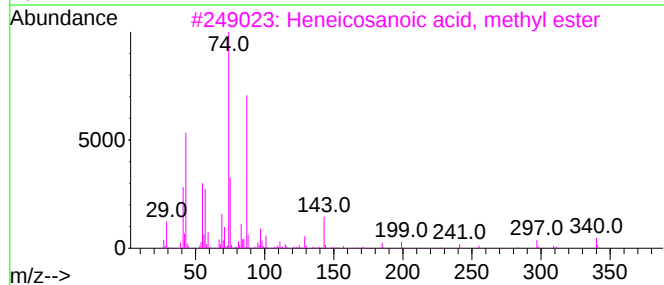
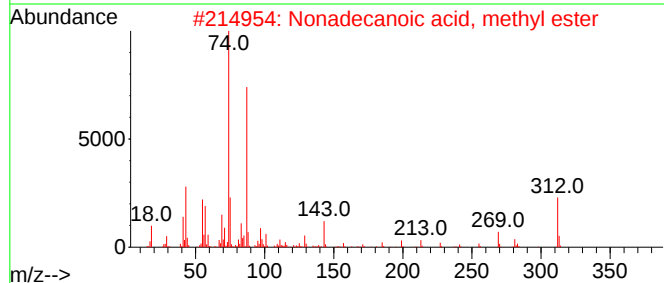
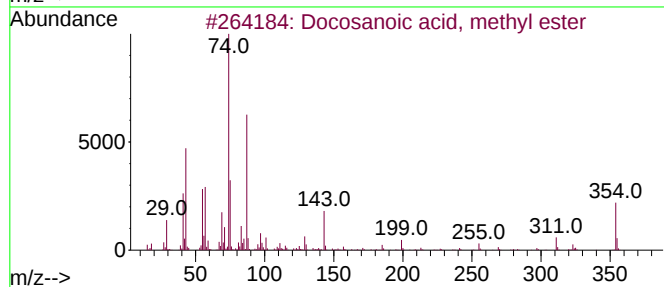
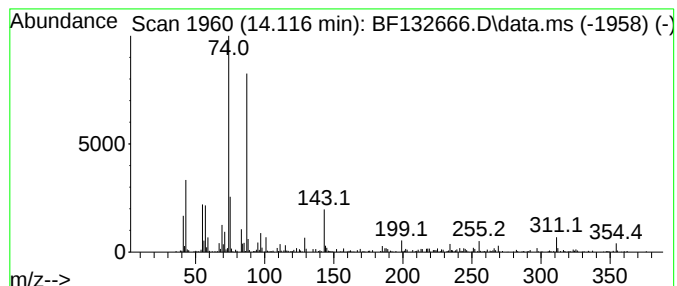
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Docosanoic acid, methyl ester Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.116	3.84 ng	267284	Chrysene-d12	14.204	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	96
2	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	91
3	Heneicosanoic acid, methyl ester	340	C22H44O2	006064-90-0	87
4	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	87
5	Octadecanoic acid, 17-methyl-, m...	312	C20H40O2	055124-97-5	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
Data File : BF132666.D
Acq On : 07 Mar 2023 00:25
Operator : CG\JU
Sample : 01820-03 2X
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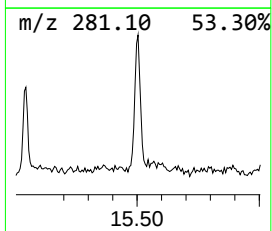
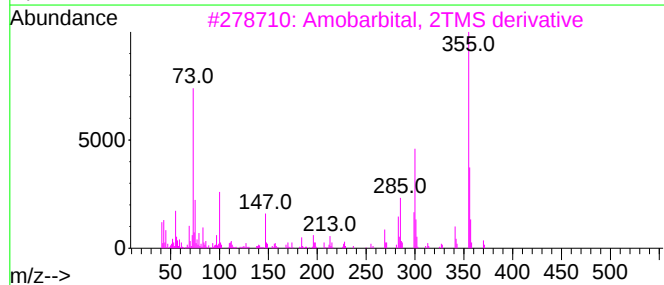
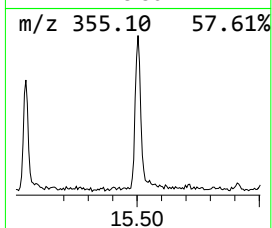
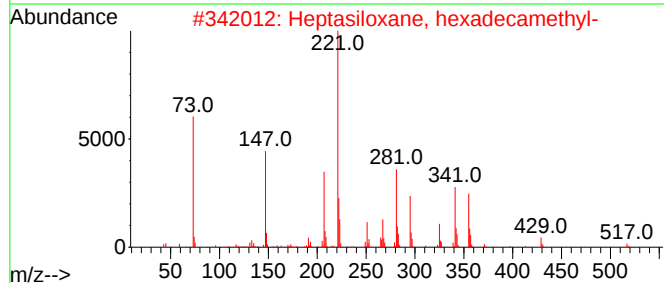
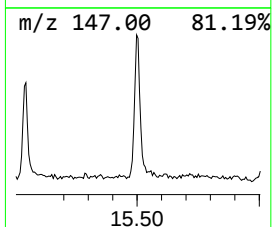
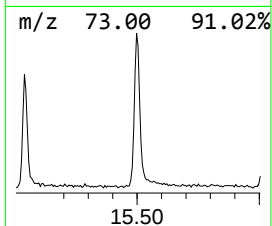
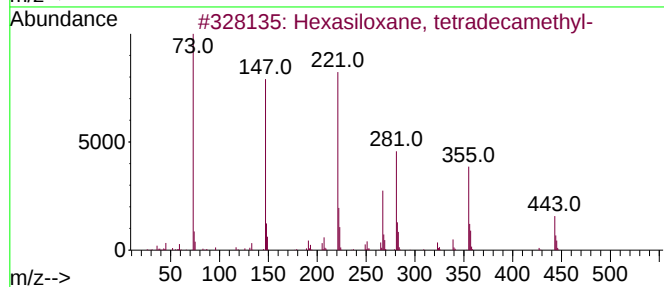
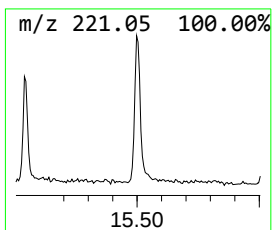
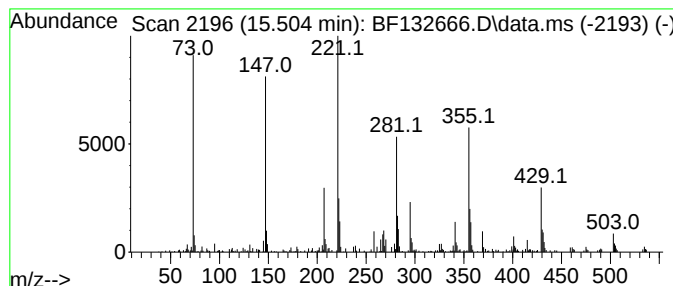
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Hexasiloxane, tetradecamethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.504	11.64 ng	521349	Perylene-d12		15.763	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-		458	C14H42O5Si6	000107-52-8	59
2	Heptasiloxane, hexadecamethyl-		532	C16H48O6Si7	000541-01-5	38
3	Amobarbital, 2TMS derivative		370	C17H34N2O3Si2	052937-67-4	15
4	2,5-Dihydroxybenzoic acid, 3TMS ...		370	C16H30O4Si3	003618-20-0	11
5	3,6-Dioxa-2,4,5,7-tetrasilaoctan...		294	C10H30O2Si4	004342-25-0	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
Data File : BF132666.D
Acq On : 07 Mar 2023 00:25
Operator : CG\JU
Sample : 01820-03 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

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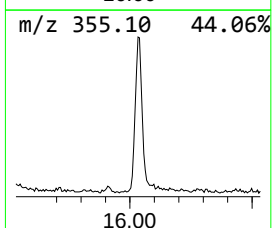
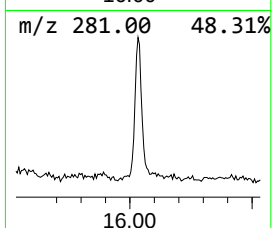
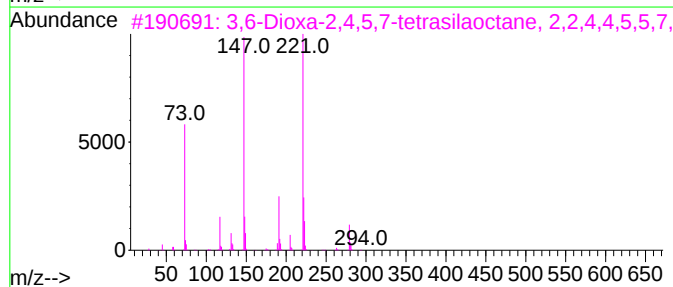
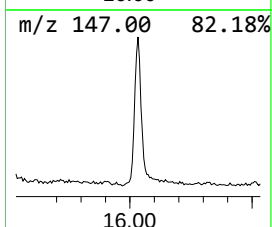
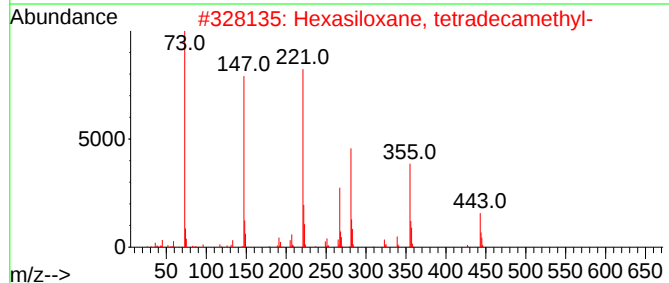
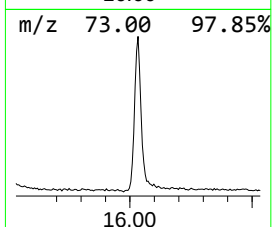
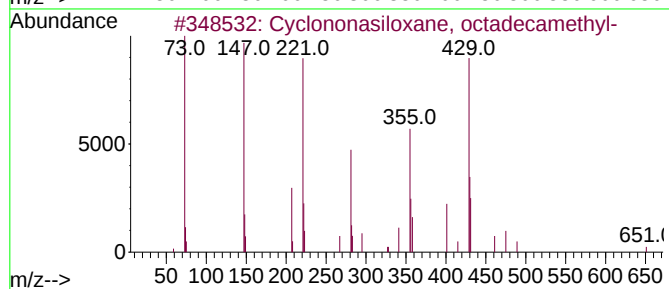
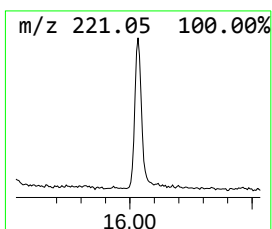
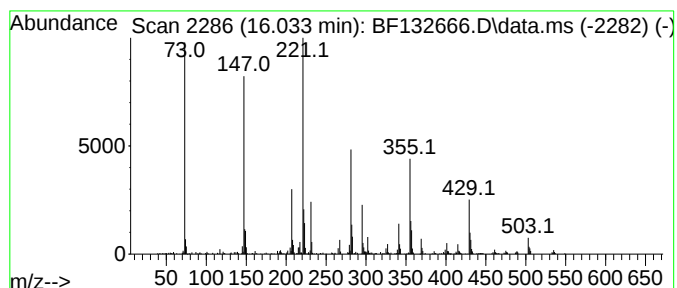
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Cyclononasiloxane, octadeca... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.033	15.22 ng	681281	Perylene-d12	15.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	86
2		Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	58
3		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	46
4		Cyclodecasiloxane, eicosamethyl-	740	C20H60O10Si10	018772-36-6	38
5		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
Data File : BF132666.D
Acq On : 07 Mar 2023 00:25
Operator : CG\JU
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HR-4-03032023

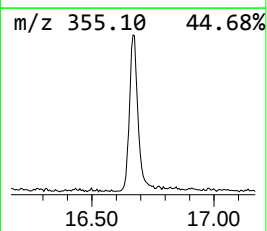
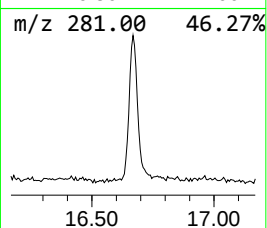
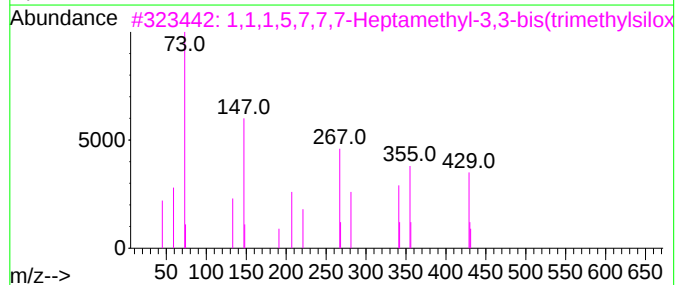
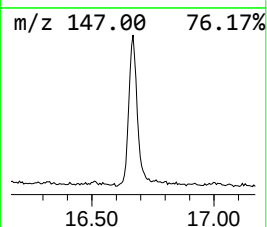
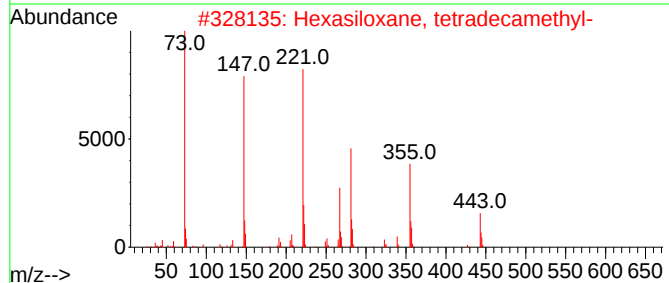
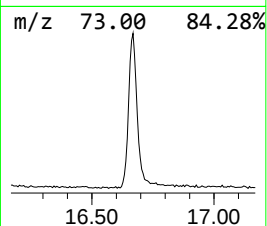
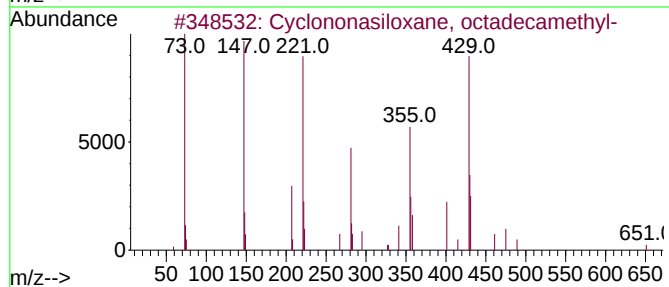
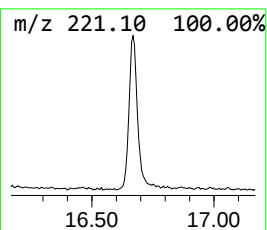
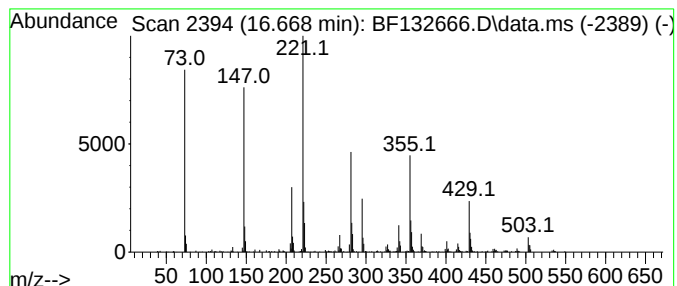
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown16.668 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.668	23.81 ng	1065930	Perylene-d12	15.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	86
2		Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
3		1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	37
4		2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	37
5		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
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Acq On : 07 Mar 2023 00:25
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Sample : 01820-03 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

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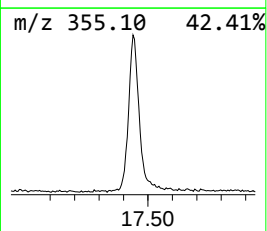
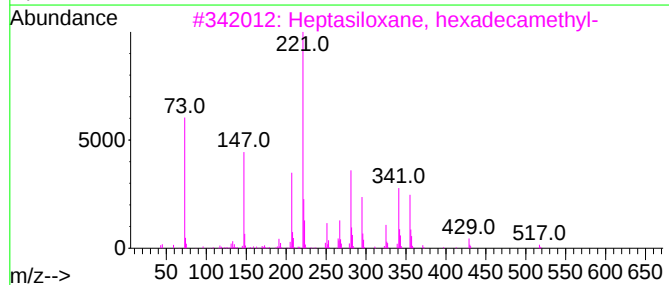
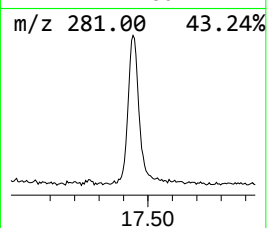
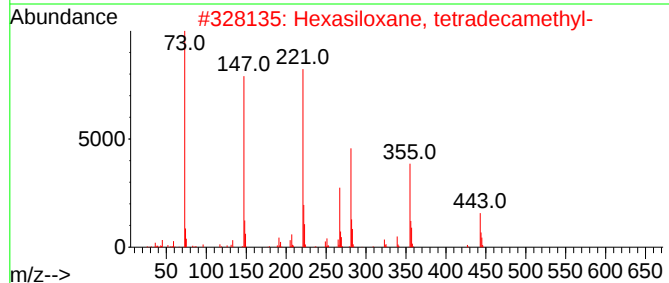
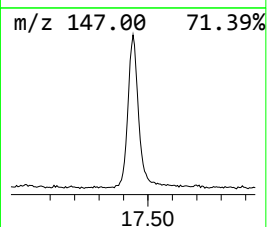
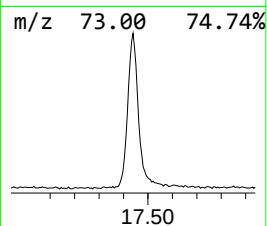
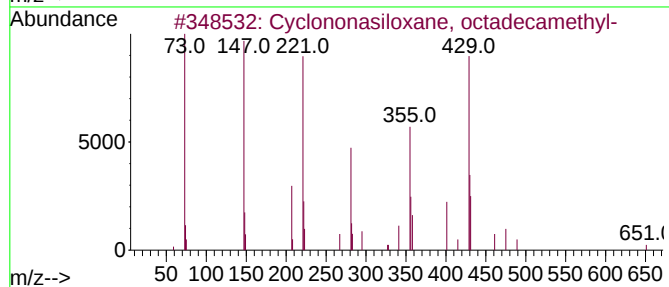
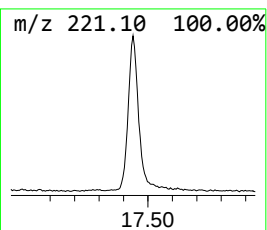
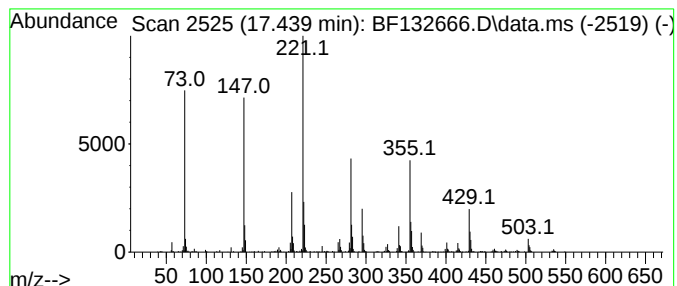
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown17.439 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.439	36.68 ng	1642010	Perylene-d12	15.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	87
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	49
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	45
4			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	38
5			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
Data File : BF132666.D
Acq On : 07 Mar 2023 00:25
Operator : CG\JU
Sample : 01820-03 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

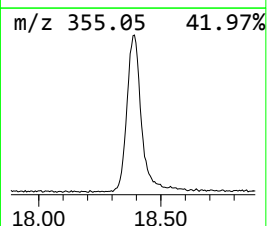
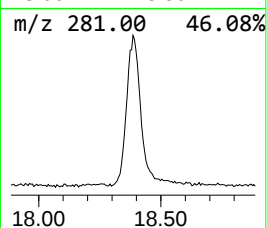
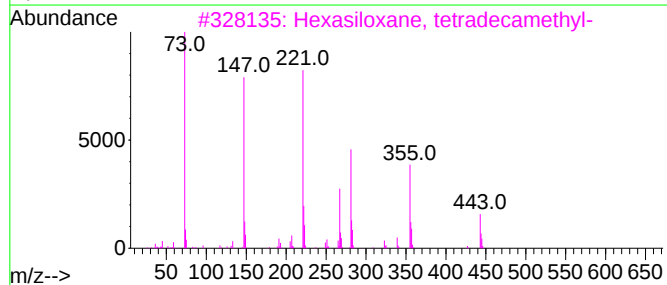
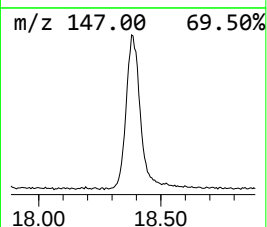
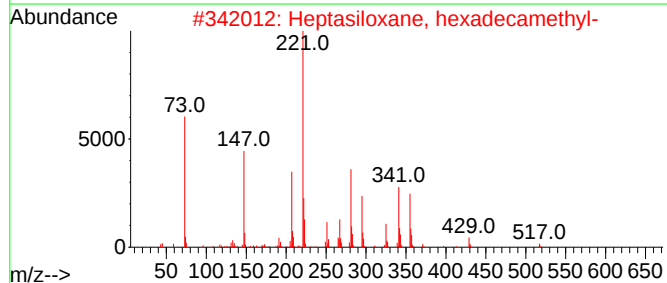
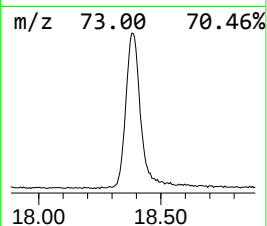
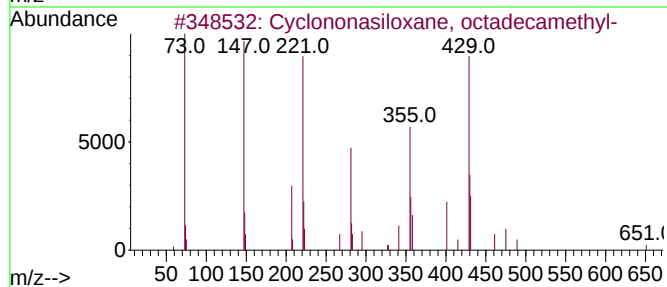
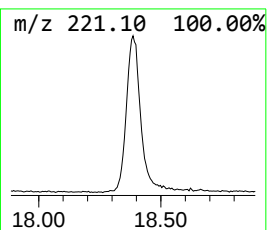
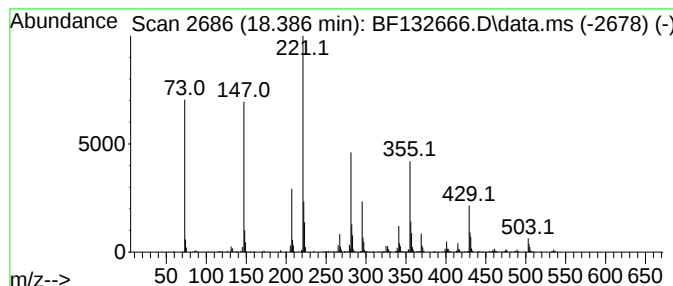
Instrument :
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ClientSampleId :
HR-4-03032023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Heptasiloxane, hexadecamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.386	50.05 ng	2240650	Perylene-d12	15.763	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	87
2	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	64
3	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	59
4	2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	32
5	1,3,5-Trisiloxane, 1,1,3,3,5,5-h...	320	C14H36O2Si3	1000458-50-5	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030623\
Data File : BF132666.D
Acq On : 07 Mar 2023 00:25
Operator : CG\JU
Sample : 01820-03 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-4-03032023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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
2-Pentanone, 4-...	5.216	12.6	ng	706206	1	6.998	1120460	20.0
Nonanoic acid, ...	9.616	2.2	ng	133968	3	10.045	1239450	20.0
Benzophenone	10.757	4.3	ng	266612	3	10.045	1239450	20.0
Hexadecanoic ac...	11.922	51.1	ng	2939440	4	11.539	1151070	20.0
n-Hexadecanoic ...	12.057	13.9	ng	802349	4	11.539	1151070	20.0
Dodecanoic acid...	12.304	6.0	ng	345923	4	11.539	1151070	20.0
9,15-Octadecadi...	12.616	150.3	ng	8649340	4	11.539	1151070	20.0
9-Octadecenoic ...	12.639	117.3	ng	6748300	4	11.539	1151070	20.0
Octadecanoic acid	12.845	5.0	ng	288481	4	11.539	1151070	20.0
Hexadecanoic ac...	13.445	3.0	ng	212644	5	14.204	1393790	20.0
unknown13.475	13.475	2.3	ng	160196	5	14.204	1393790	20.0
unknown13.516	13.516	2.3	ng	160817	5	14.204	1393790	20.0
2-(1-Hydroxycyc...	13.874	4.6	ng	318457	5	14.204	1393790	20.0
Docosanoic acid...	14.116	3.8	ng	267284	5	14.204	1393790	20.0
Hexasiloxane, t...	15.504	11.6	ng	521349	6	15.763	895419	20.0
Cyclononasiloxa...	16.033	15.2	ng	681281	6	15.763	895419	20.0
unknown16.668	16.668	23.8	ng	1065930	6	15.763	895419	20.0
unknown17.439	17.439	36.7	ng	1642010	6	15.763	895419	20.0
Heptasiloxane, ...	18.386	50.0	ng	2240650	6	15.763	895419	20.0