

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
 Data File : BF132741.D
 Acq On : 10 Mar 2023 14:59
 Operator : CG\JU
 Sample : 01853-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20230168-COMPOSITE-2-ELUTRIATE

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: BF132741.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.610	340	344	349	rVB	76691	78171	1.04%	0.171%
2	5.210	441	446	457	rVB	1408996	1497691	19.84%	3.281%
3	5.610	510	514	524	rBV	3064955	2825903	37.43%	6.191%
4	5.993	575	579	583	rBV	144048	120844	1.60%	0.265%
5	6.604	680	683	695	rVB	2130404	1890732	25.05%	4.142%
6	6.975	743	746	750	rBV	1599140	1380806	18.29%	3.025%
7	7.545	833	843	846	rBV	3984248	4363551	57.80%	9.559%
8	7.710	867	871	874	rVB	120884	100981	1.34%	0.221%
9	8.263	961	965	968	rBV	2229757	1790209	23.72%	3.922%
10	8.945	1078	1081	1084	rBV	137725	126042	1.67%	0.276%
11	9.345	1143	1149	1152	rBV	7281905	7548826	100.00%	16.537%
12	9.404	1156	1159	1163	rBV	142505	114178	1.51%	0.250%
13	10.022	1261	1264	1268	rVB	2272226	2078688	27.54%	4.554%
14	10.116	1277	1280	1283	rBV	159464	118294	1.57%	0.259%
15	10.739	1383	1386	1389	rVB	710447	554907	7.35%	1.216%
16	10.822	1395	1400	1403	rBV	5015718	4822011	63.88%	10.563%
17	11.045	1436	1438	1443	rBV	96944	83021	1.10%	0.182%
18	11.157	1453	1457	1463	rVB7	55892	99414	1.32%	0.218%
19	11.522	1515	1519	1522	rBV	2580421	2161752	28.64%	4.736%
20	11.616	1532	1535	1538	rVB	156717	124824	1.65%	0.273%
21	11.675	1541	1545	1548	rBV	236059	223178	2.96%	0.489%
22	12.028	1600	1605	1610	rBV	573237	771866	10.22%	1.691%
23	12.186	1628	1632	1634	rBV	195355	201371	2.67%	0.441%
24	12.222	1635	1638	1640	rBV	74038	92934	1.23%	0.204%
25	12.822	1730	1740	1751	rVB3	161502	367611	4.87%	0.805%
26	13.116	1785	1790	1793	rBV	7096662	6852769	90.78%	15.012%
27	13.204	1799	1805	1813	rVB2	202200	399505	5.29%	0.875%
28	13.322	1822	1825	1828	rBV	75039	86392	1.14%	0.189%
29	13.363	1828	1832	1840	rVB5	92646	217698	2.88%	0.477%
30	13.892	1916	1922	1928	rVB	249970	422341	5.59%	0.925%
31	14.004	1937	1941	1959	rBV	463661	913000	12.09%	2.000%
32	14.180	1967	1971	1975	rVB	1437121	1242423	16.46%	2.722%
33	14.445	2012	2016	2023	rVB	238847	312847	4.14%	0.685%
34	14.974	2101	2106	2110	rVB2	137404	216774	2.87%	0.475%
35	15.027	2112	2115	2120	rVB	128476	138216	1.83%	0.303%
36	15.557	2202	2205	2212	rVB	103362	175762	2.33%	0.385%

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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	15.721	2228	2233	2241	rVB	851670	1132804	15.01%	2.482%
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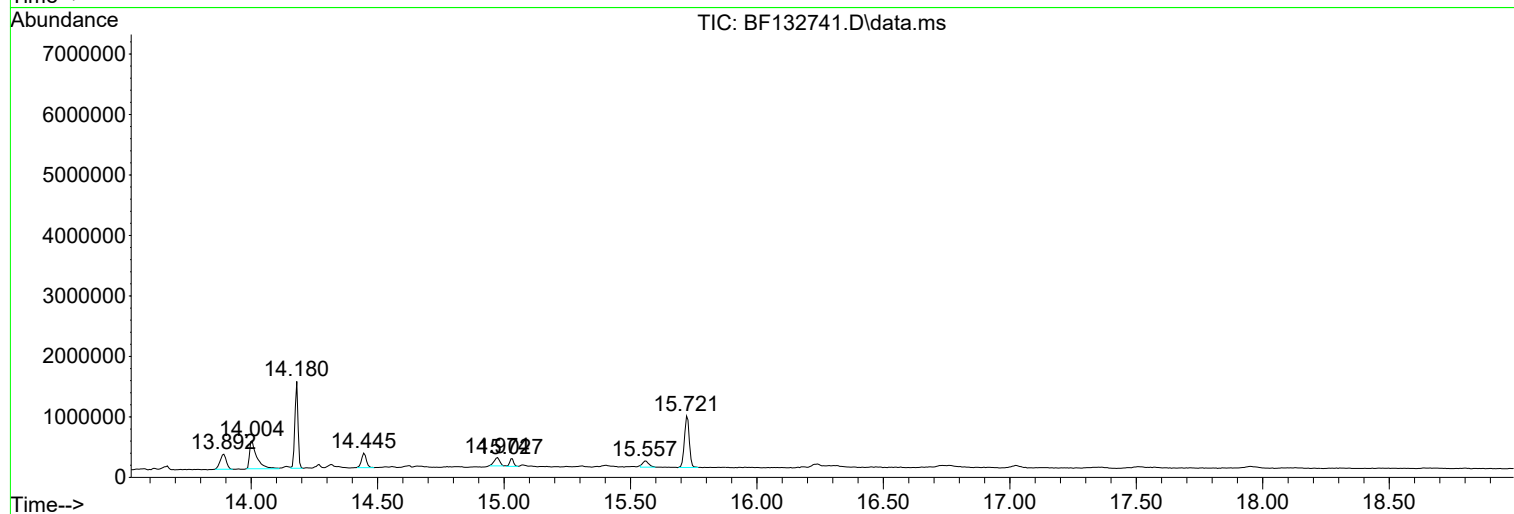
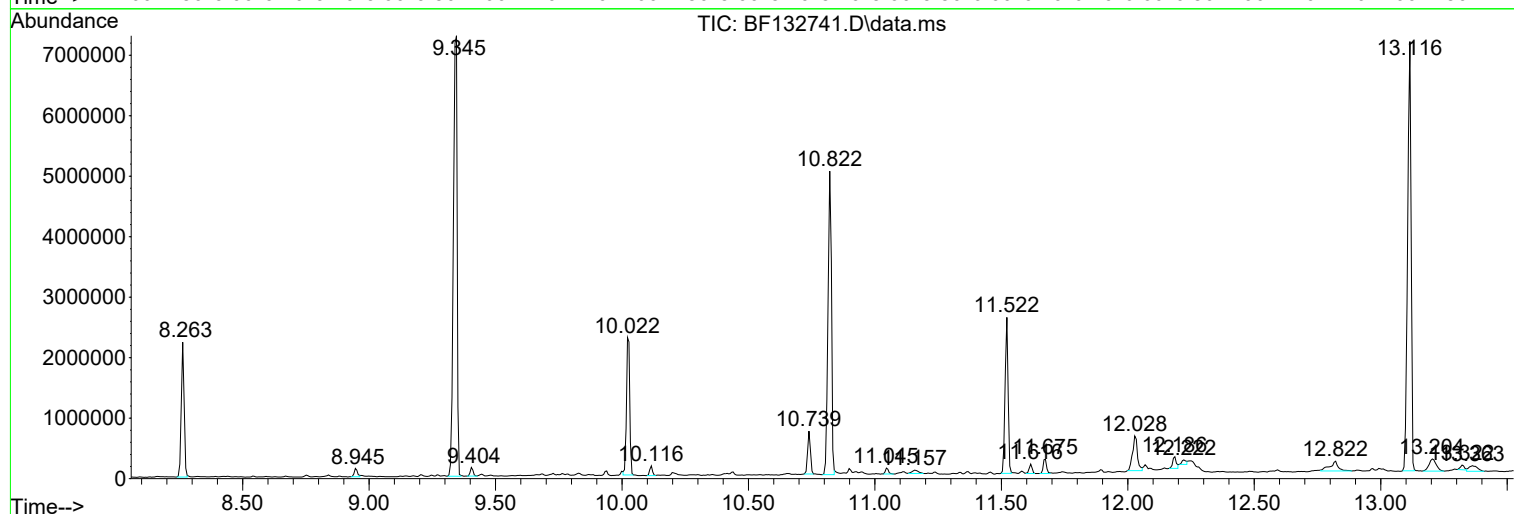
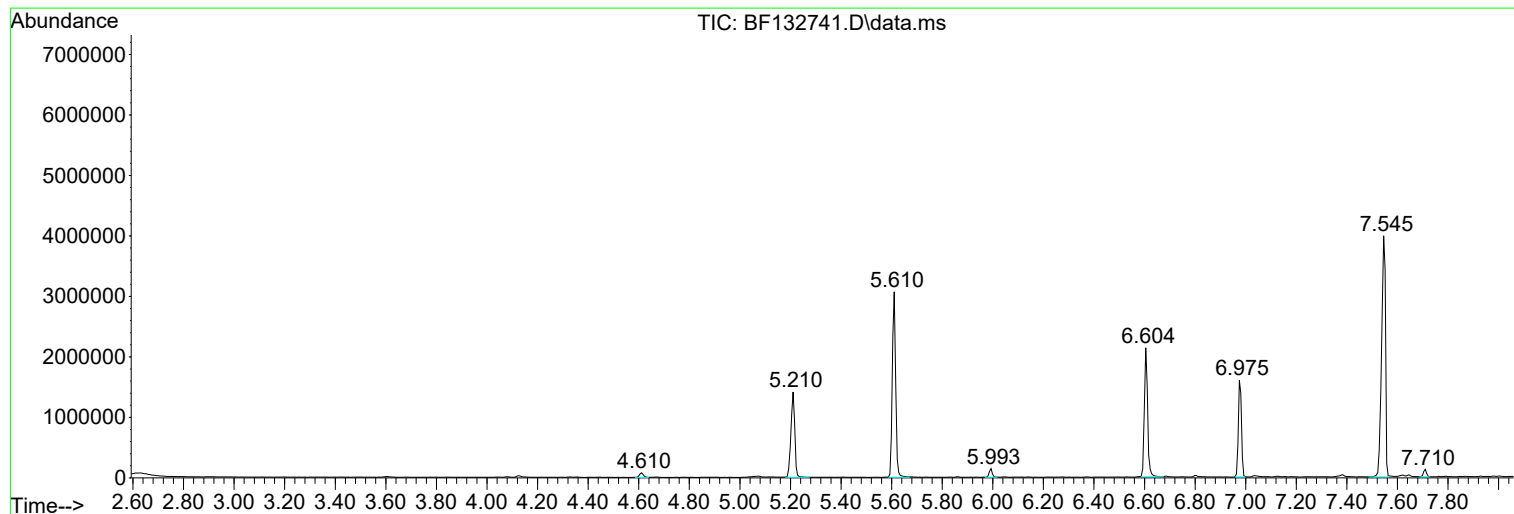
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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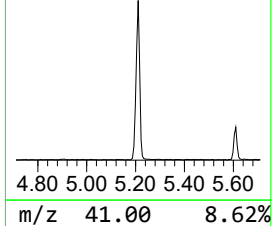
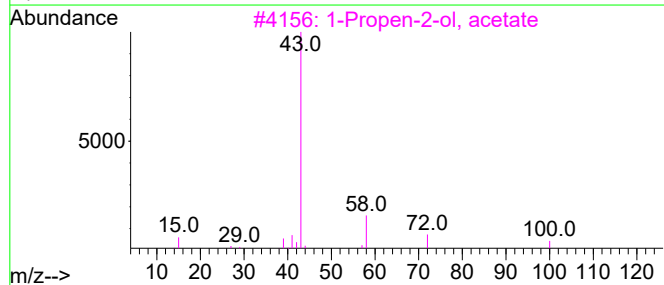
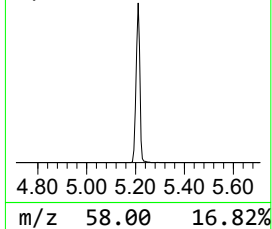
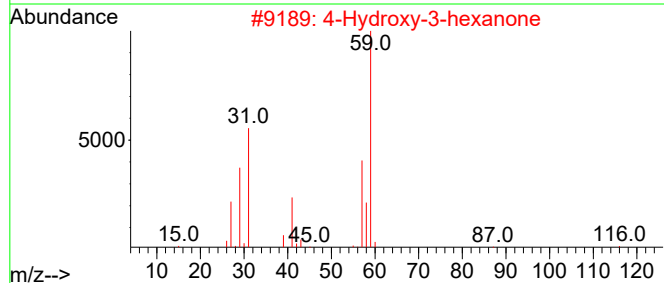
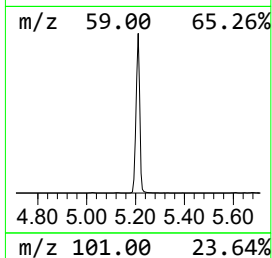
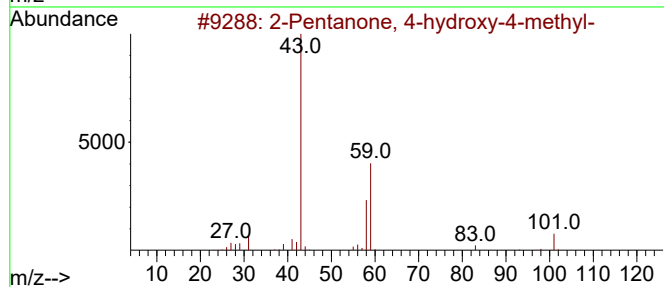
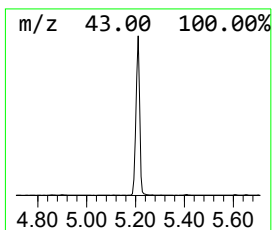
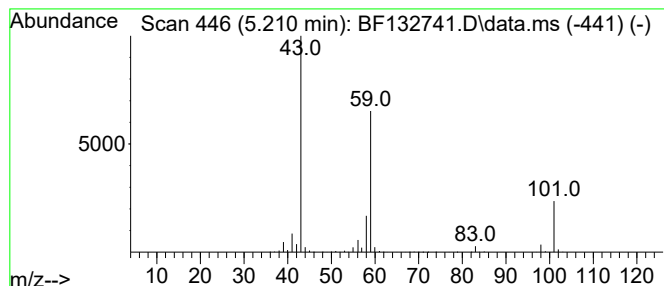
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.210	21.69 ng	1497690	1,4-Dichlorobenzene-d4	6.975	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Acetone	58	C3H6O	000067-64-1	9



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Instrument :
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20230168-COMPOSITE-2-ELUTRIATE

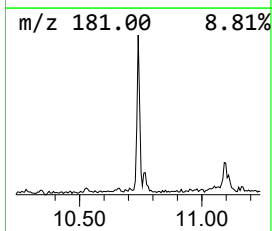
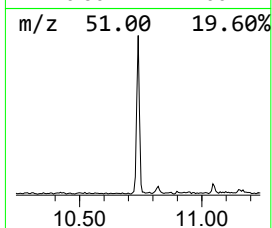
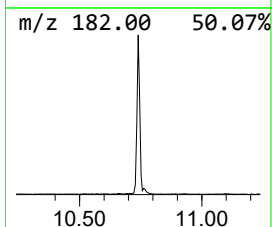
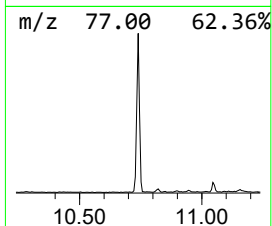
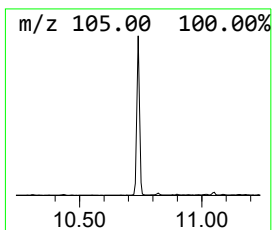
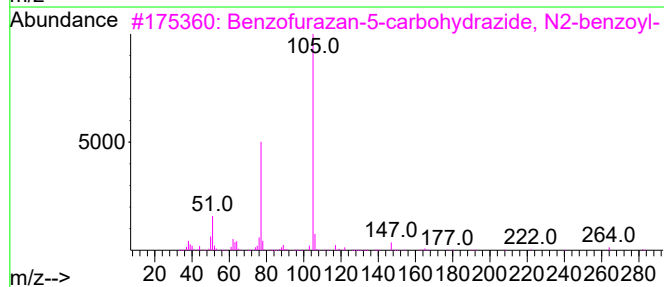
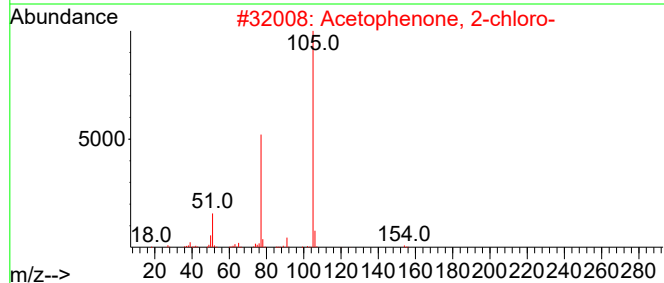
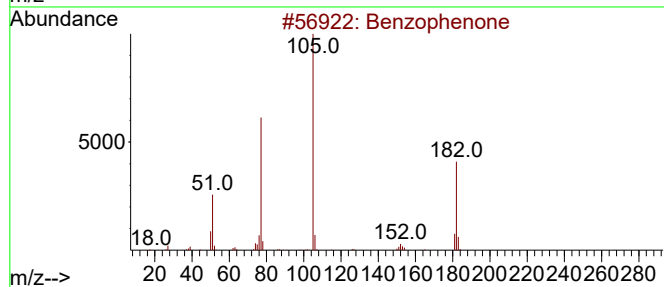
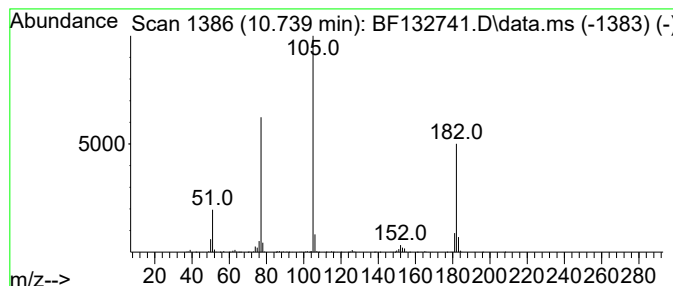
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.739	5.34 ng	554907	Acenaphthene-d10	10.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			Benzofurazan-5-carbohydrazide, N...	282	C14H10N4O3	1000272-94-4	47
4			.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	47
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47



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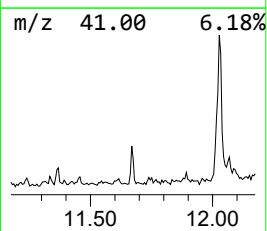
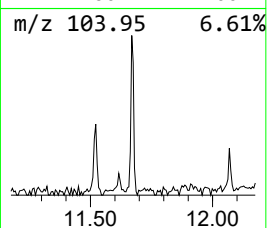
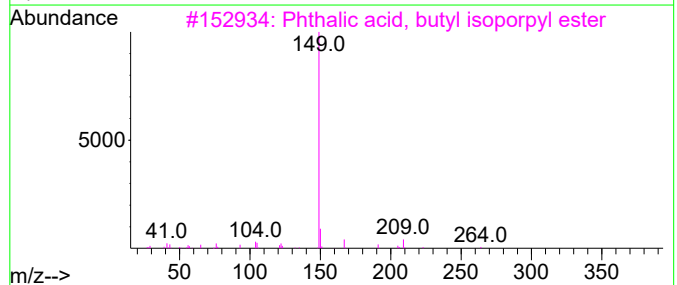
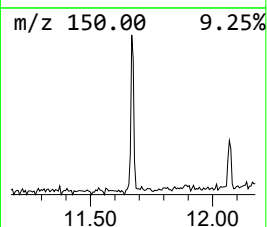
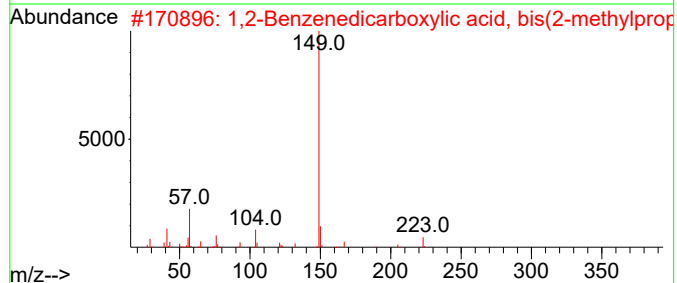
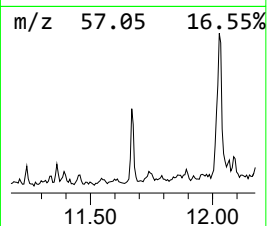
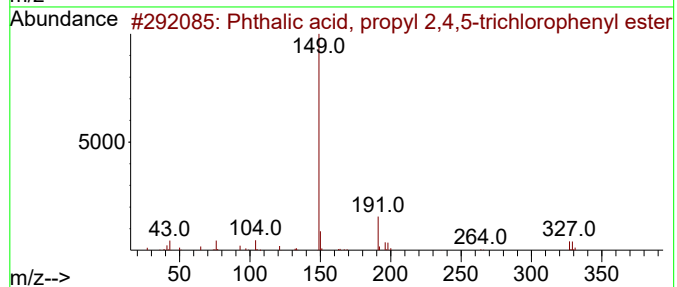
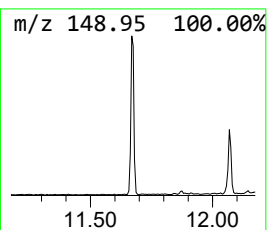
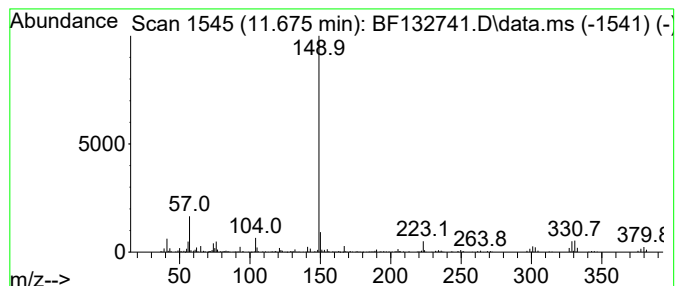
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Phthalic acid, propyl 2,4,5... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.675	2.06 ng	223178	Phenanthrene-d10	11.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, propyl 2,4,5-tric...	386	C17H13Cl3O4	1000357-04-2	72
2			1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	68
3			Phthalic acid, butyl isopropyl e...	264	C15H20O4	1000314-99-8	64
4			Phthalic acid, ethyl pentyl ester	264	C15H20O4	1000308-93-6	64
5			Phthalic acid, 3,4-dichloropheny...	408	C21H22Cl2O4	1000315-27-6	59



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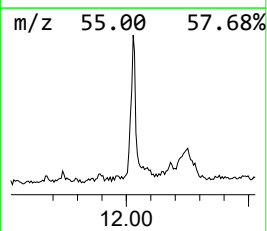
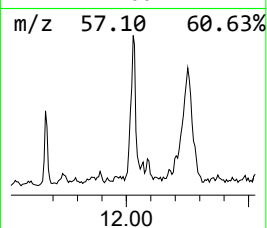
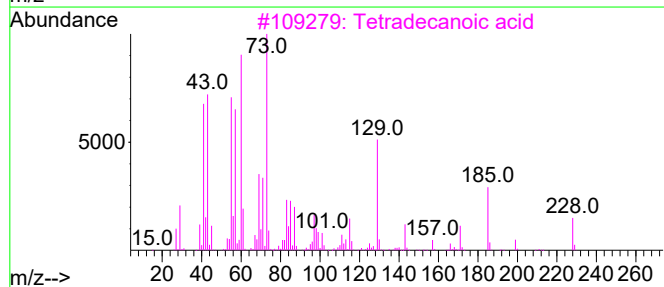
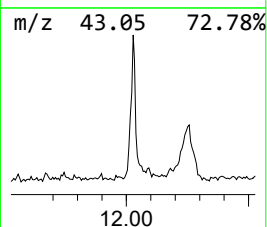
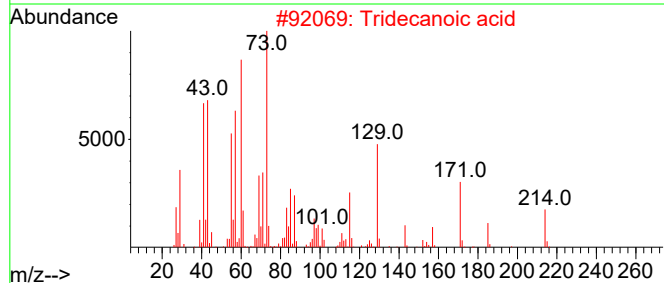
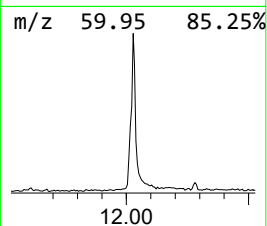
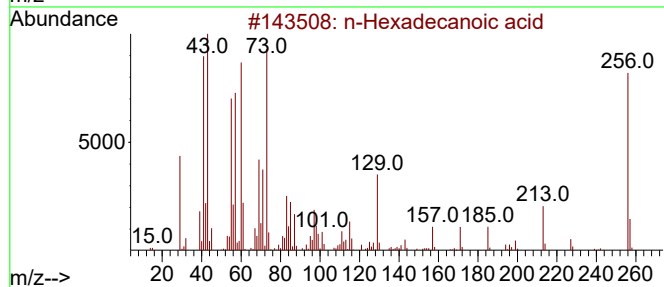
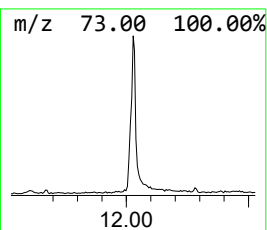
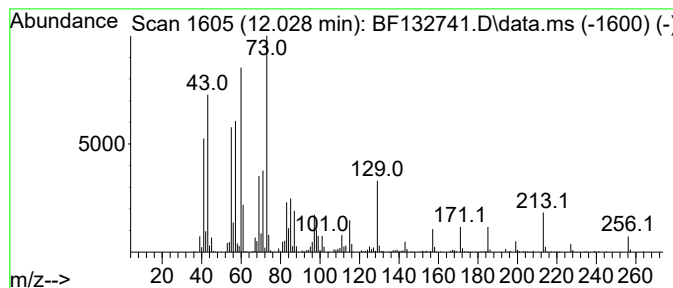
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.028	7.14 ng	771866	Phenanthrene-d10	11.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	96
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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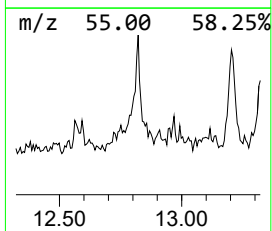
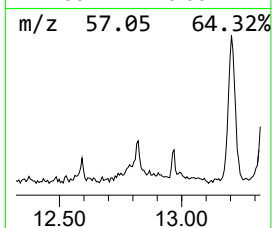
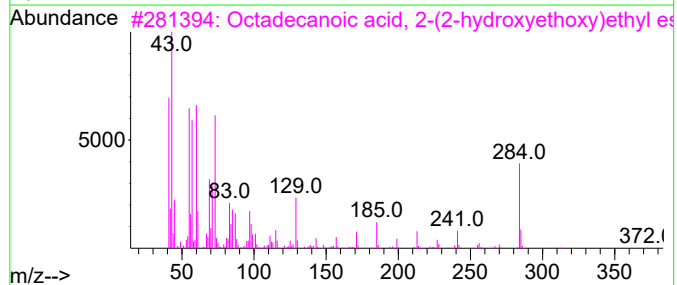
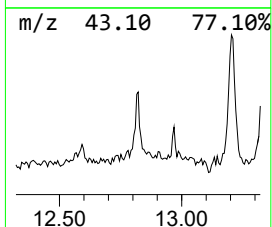
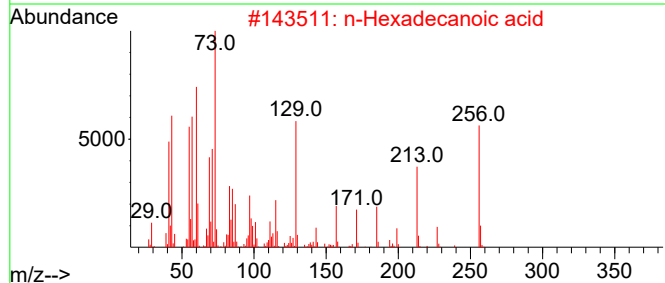
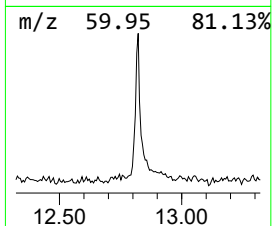
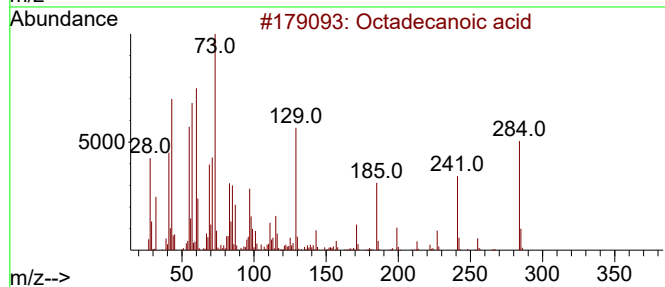
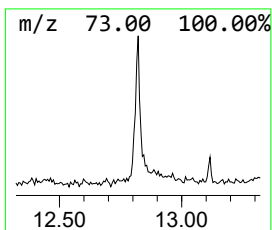
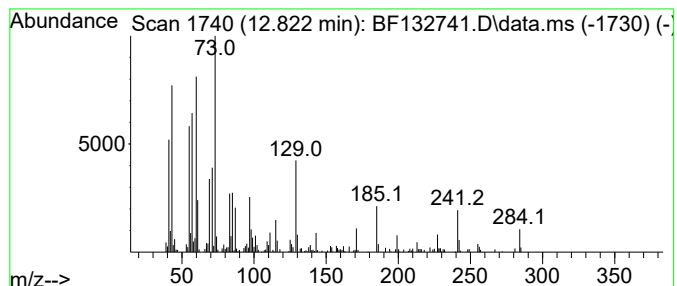
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.822	3.40 ng	367611	Phenanthrene-d10	11.522

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			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
Data File : BF132741.D
Acq On : 10 Mar 2023 14:59
Operator : CG\JU
Sample : 01853-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
20230168-COMPOSITE-2-ELUTRIATE

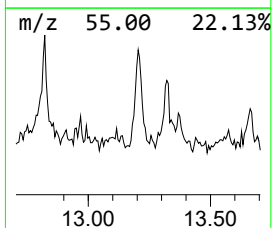
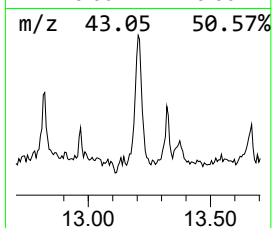
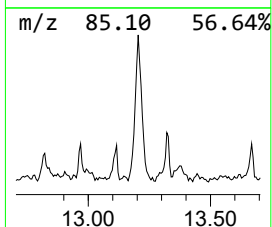
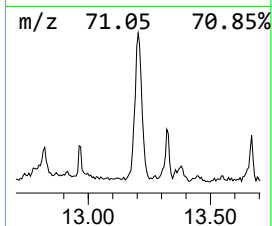
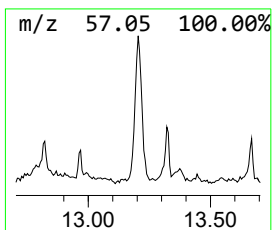
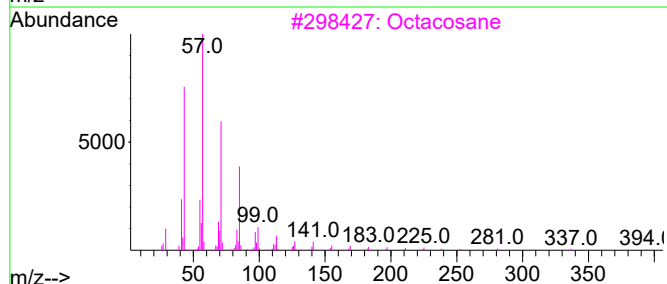
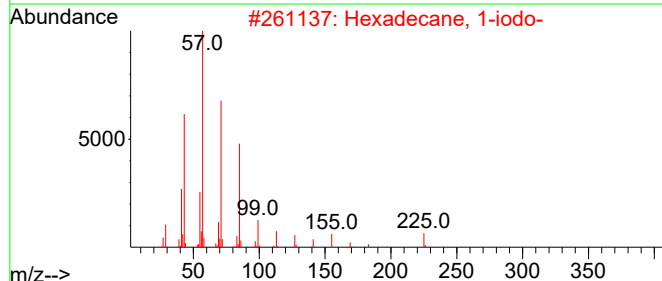
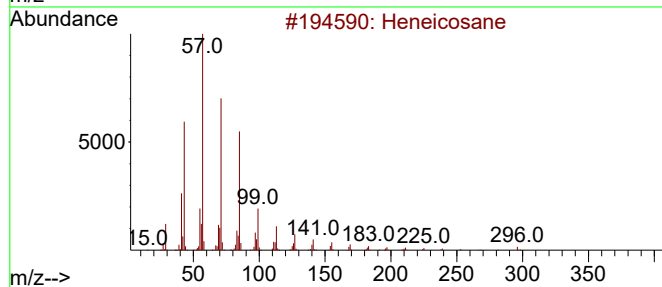
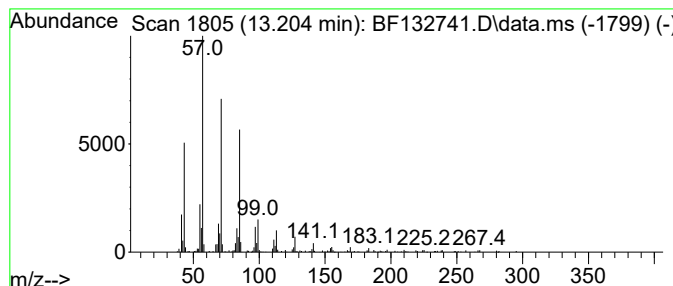
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.204	6.43 ng	399505	Chrysene-d12	14.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87
3			Octacosane	394	C28H58	000630-02-4	86
4			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
5			Octadecane	254	C18H38	000593-45-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
Data File : BF132741.D
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Operator : CG\JU
Sample : 01853-04
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Instrument :
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ClientSampleId :
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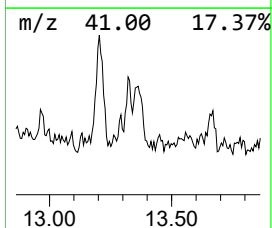
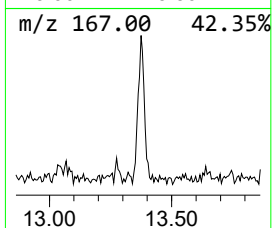
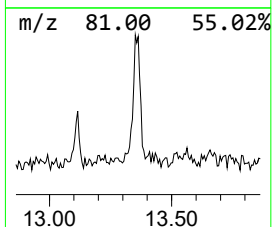
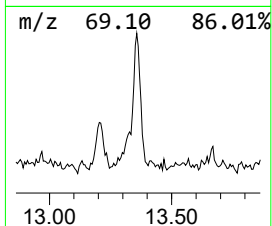
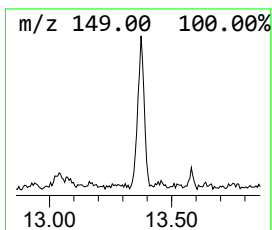
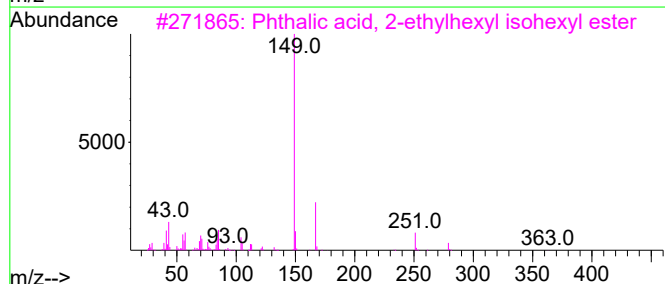
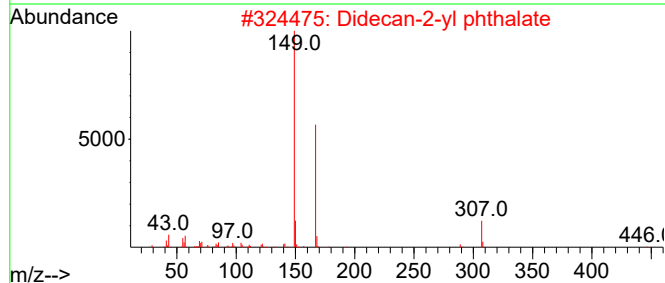
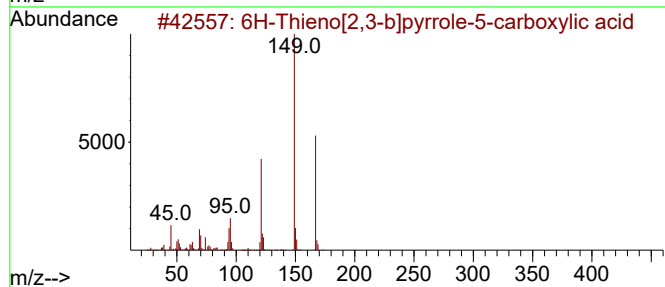
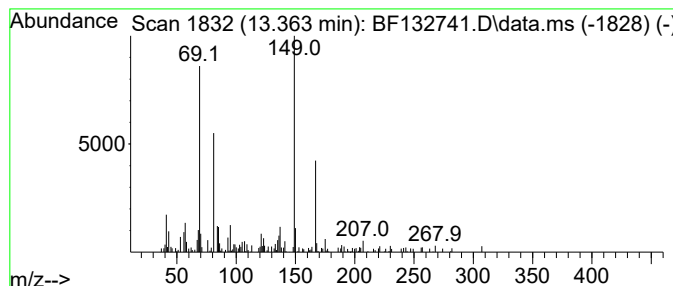
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown13.363 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.363	3.50 ng	217698	Chrysene-d12	14.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6H-Thieno[2,3-b]pyrrole-5-carbox...	167	C7H5N02S	051856-25-8	46
2			Didecan-2-yl phthalate	446	C28H46O4	028029-89-2	38
3			Phthalic acid, 2-ethylhexyl isoh...	362	C22H34O4	1000308-98-5	38
4			Phthalic acid, monocyclohexyl ester	248	C14H16O4	007517-36-4	38
5			Phthalic acid, ethyl 4-methylpen...	278	C16H22O4	1000356-87-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
Data File : BF132741.D
Acq On : 10 Mar 2023 14:59
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Sample : 01853-04
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ClientSampleId :
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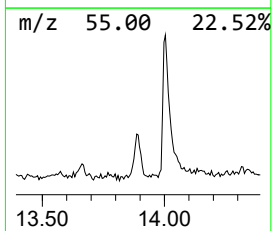
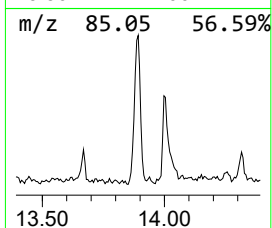
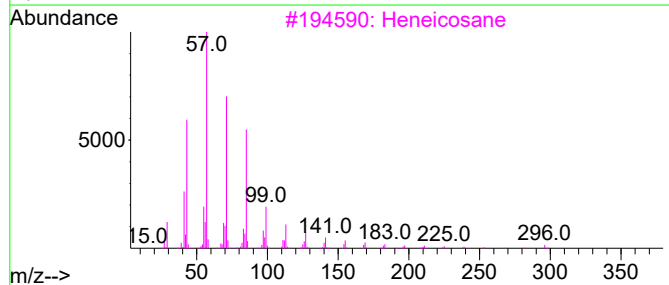
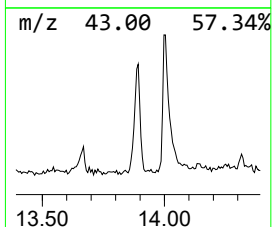
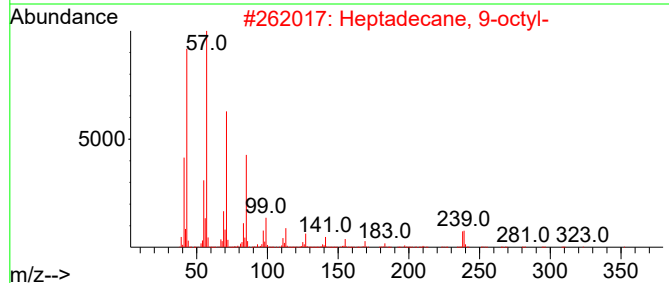
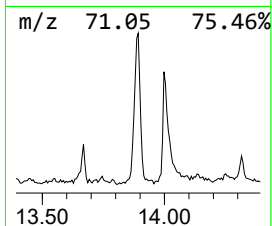
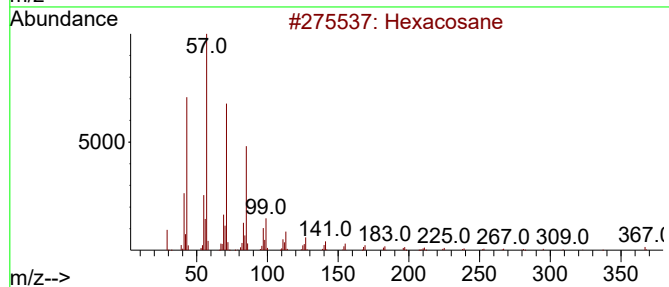
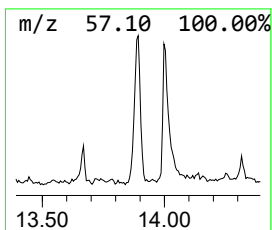
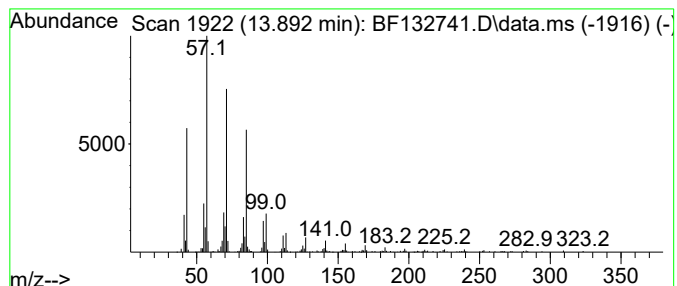
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	6.80 ng	422341	Chrysene-d12	14.180

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
Data File : BF132741.D
Acq On : 10 Mar 2023 14:59
Operator : CG\JU
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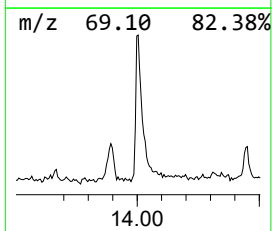
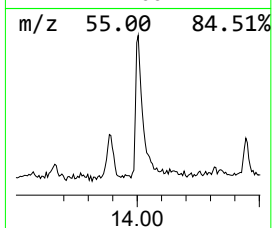
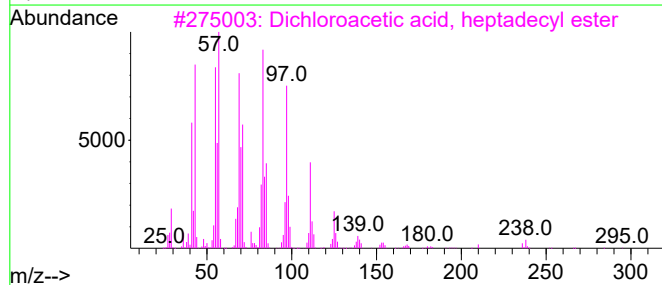
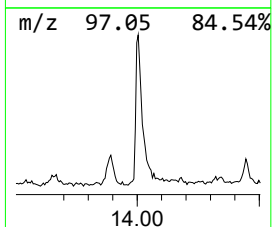
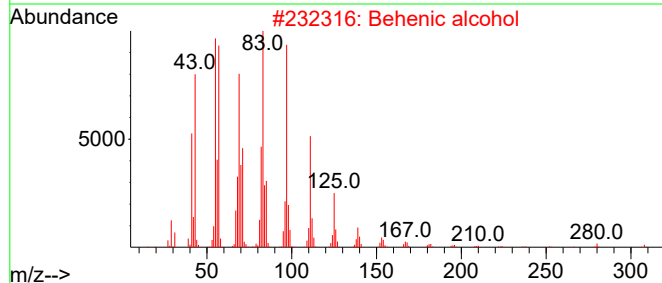
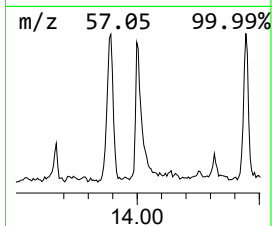
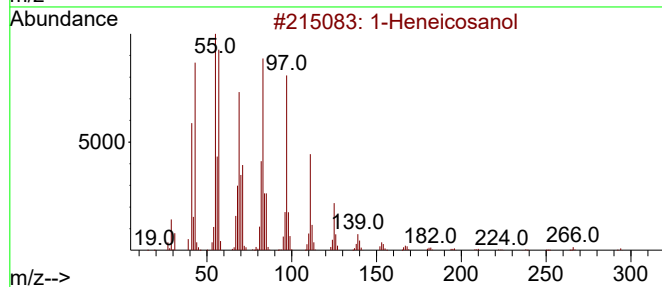
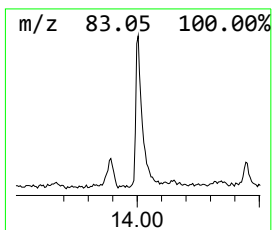
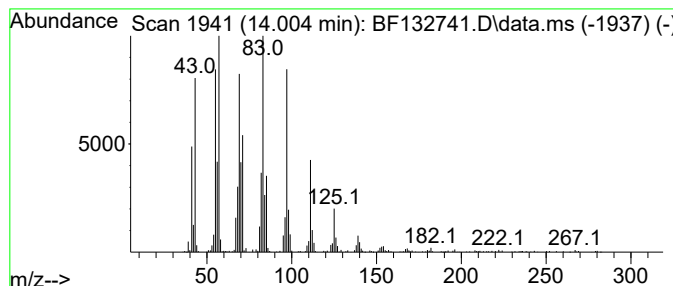
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	14.70 ng	913000	Chrysene-d12	14.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	94
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
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Sample : 01853-04
Misc :
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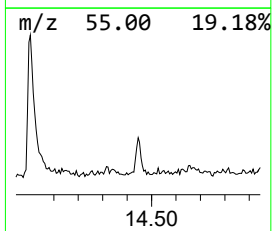
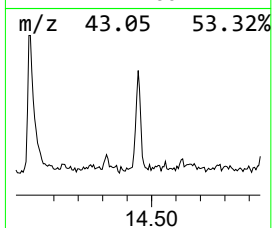
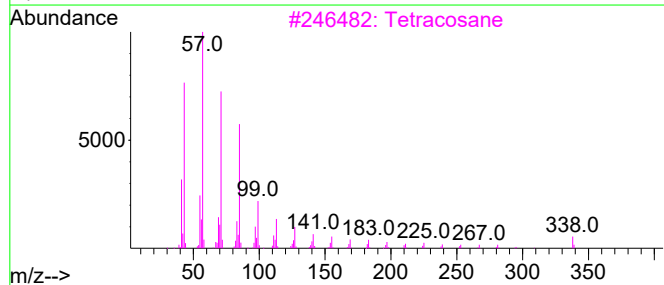
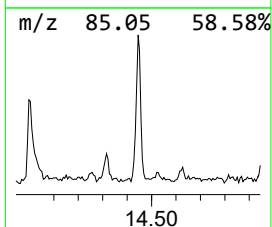
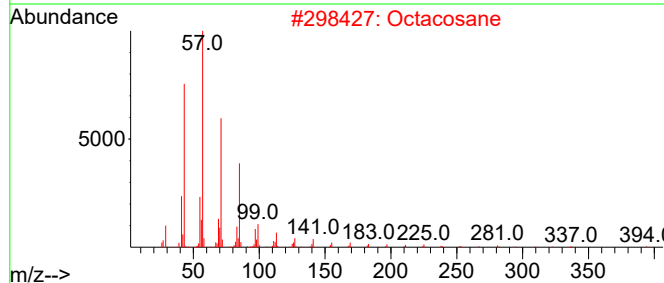
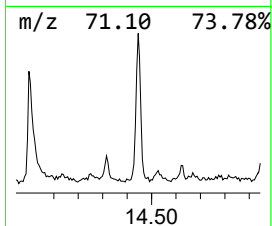
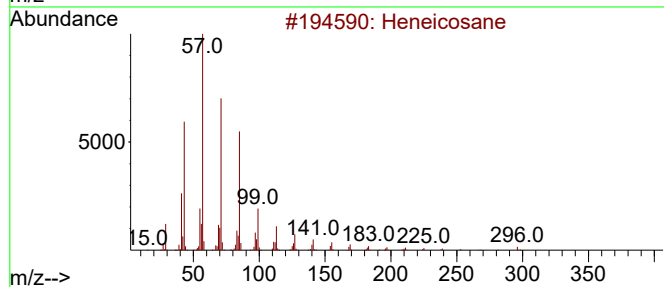
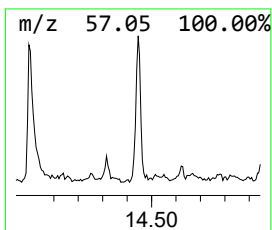
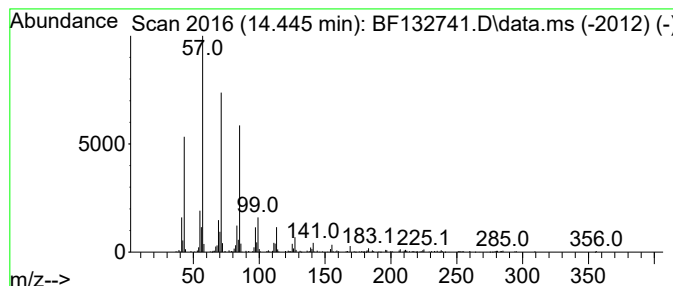
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.445	5.04 ng	312847	Chrysene-d12		14.180	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Tetracosane		338	C24H50	000646-31-1	91
4	Eicosane		282	C20H42	000112-95-8	91
5	Octacosane, 2-methyl-		408	C29H60	001560-98-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
Data File : BF132741.D
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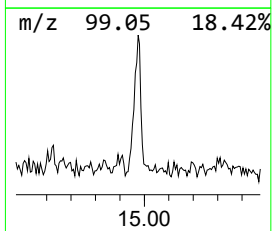
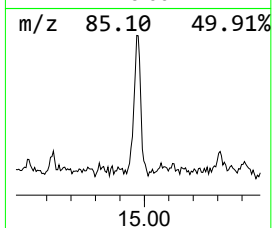
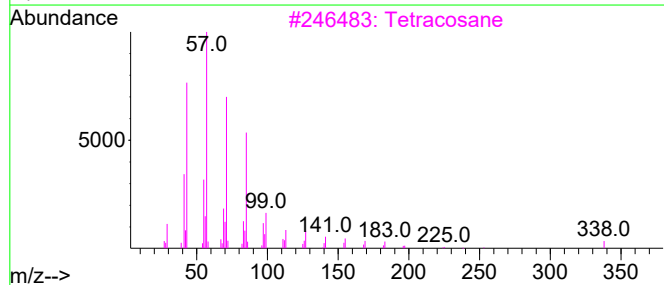
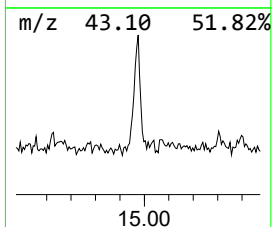
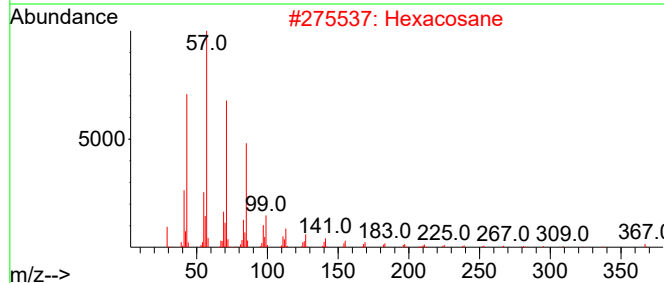
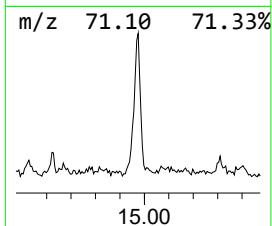
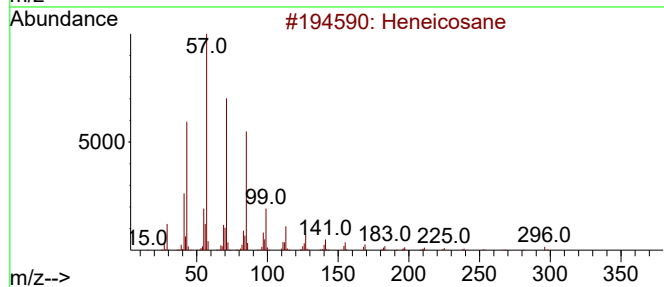
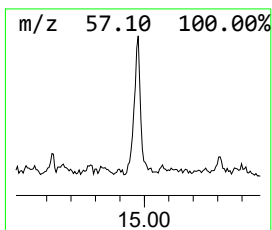
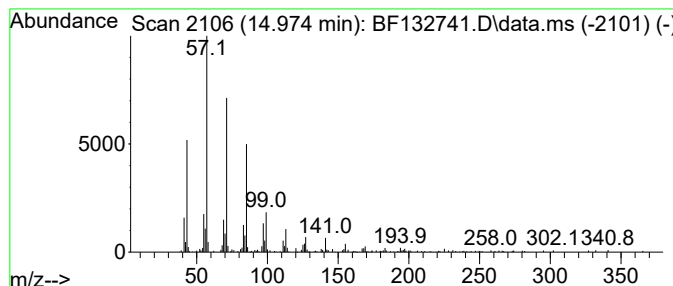
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	3.83 ng	216774	Perylene-d12	15.721

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Tetracosane	338	C24H50	000646-31-1	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Hentriacontane	437	C31H64	000630-04-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
Data File : BF132741.D
Acq On : 10 Mar 2023 14:59
Operator : CG\JU
Sample : 01853-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230168-COMPOSITE-2-ELUTRIATE

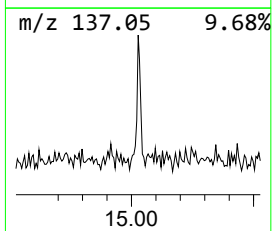
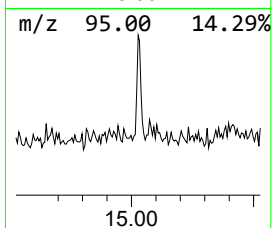
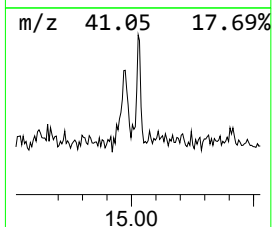
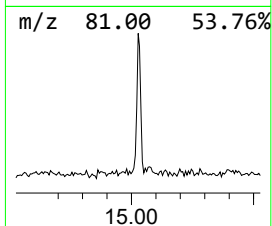
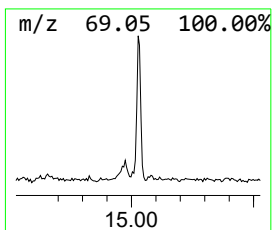
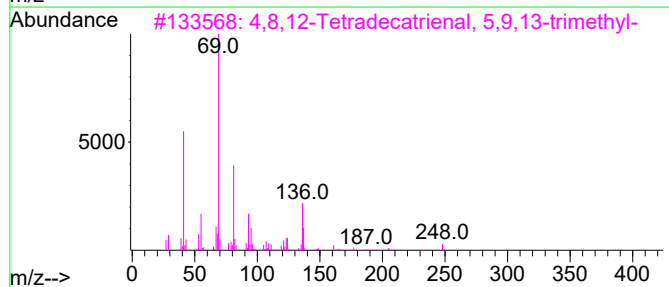
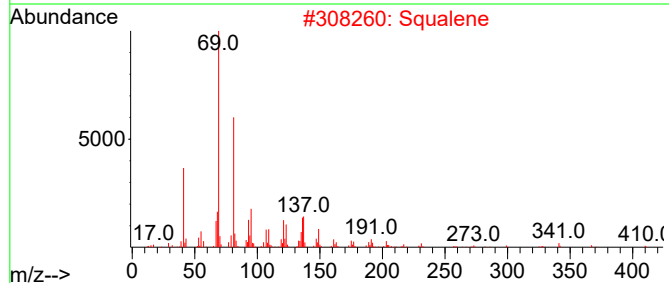
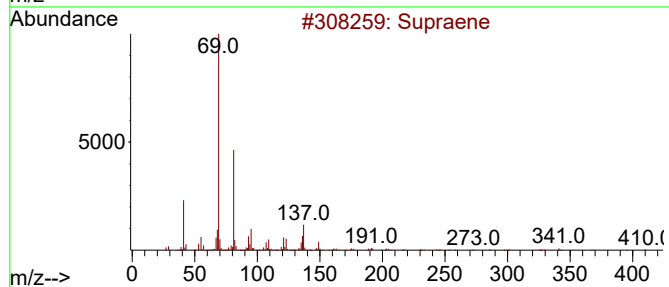
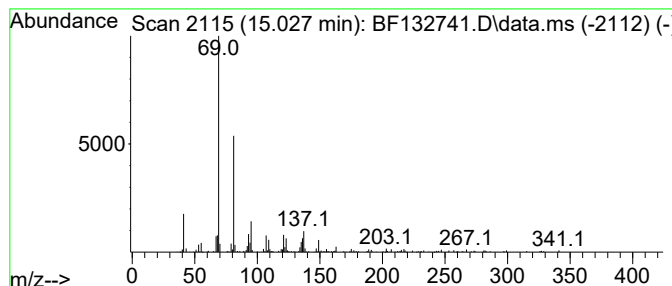
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Supraene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.027	2.44 ng	138216	Perylene-d12	15.721

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	90
2			Squalene	410	C30H50	000111-02-4	83
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4			(2E,6E)-3,7,11-Trimethyldodeca-2...	404	C27H48O2	078368-58-8	72
5			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
Data File : BF132741.D
Acq On : 10 Mar 2023 14:59
Operator : CG\JU
Sample : 01853-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230168-COMPOSITE-2-ELUTRIATE

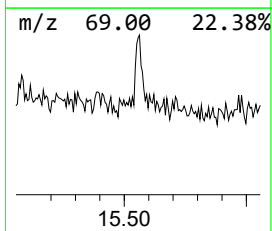
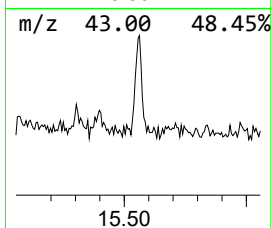
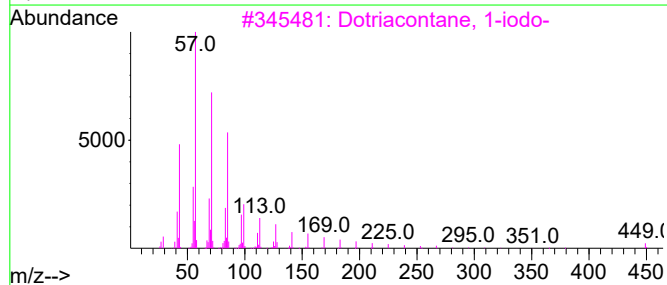
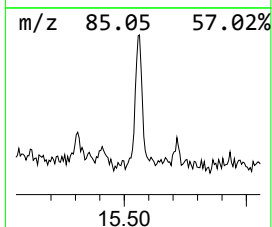
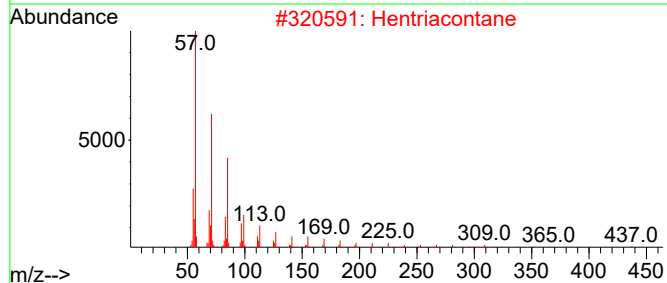
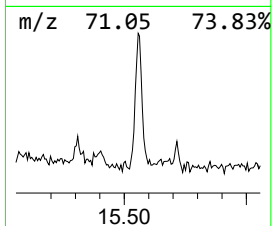
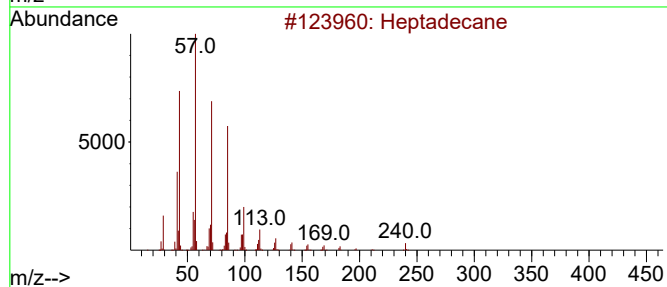
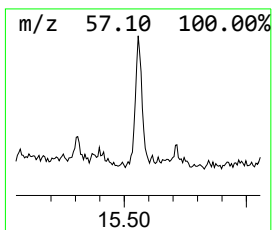
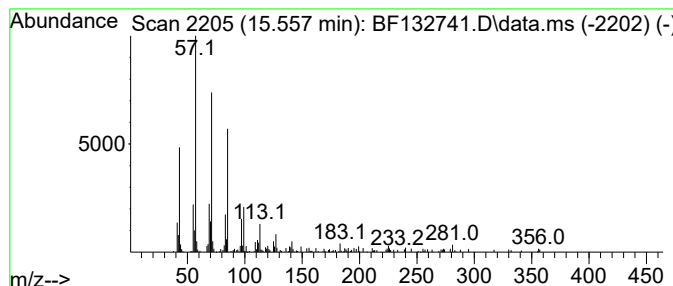
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.557	3.10 ng	175762	Perylene-d12	15.721

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	93
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
4		Pentacosane	352	C25H52	000629-99-2	90
5		Hexadecane, 2-methyl-	240	C17H36	001560-92-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
Data File : BF132741.D
Acq On : 10 Mar 2023 14:59
Operator : CG\JU
Sample : 01853-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230168-COMPOSITE-2-ELUTRIATE

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-...	5.210	21.7	ng	1497690	1	6.975	1380810	20.0
Benzophenone	10.739	5.3	ng	554907	3	10.022	2078690	20.0
Phthalic acid, ...	11.675	2.1	ng	223178	4	11.522	2161750	20.0
n-Hexadecanoic ...	12.028	7.1	ng	771866	4	11.522	2161750	20.0
Octadecanoic acid	12.822	3.4	ng	367611	4	11.522	2161750	20.0
Heneicosane	13.204	6.4	ng	399505	5	14.180	1242420	20.0
unknown13.363	13.363	3.5	ng	217698	5	14.180	1242420	20.0
Hexacosane	13.892	6.8	ng	422341	5	14.180	1242420	20.0
1-Heneicosanol	14.004	14.7	ng	913000	5	14.180	1242420	20.0
Octacosane	14.445	5.0	ng	312847	5	14.180	1242420	20.0
Tetracosane	14.974	3.8	ng	216774	6	15.721	1132800	20.0
Supraene	15.027	2.4	ng	138216	6	15.721	1132800	20.0
Heptadecane	15.557	3.1	ng	175762	6	15.721	1132800	20.0