

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022323\
 Data File : BF132520.D
 Acq On : 23 Feb 2023 14:58
 Operator : CG\JU
 Sample : 01657-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-17-SB01

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: BF132520.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.248	404	410	420	rVB	1398519	1686896	44.32%	5.416%
2	5.637	472	476	480	rBV	3169906	3158235	82.98%	10.141%
3	6.636	641	646	649	rBV	3474523	3171376	83.33%	10.183%
4	7.007	705	709	712	rBV	1364693	1057791	27.79%	3.396%
5	7.572	800	805	808	rBV	2330935	2112079	55.50%	6.782%
6	8.295	924	928	931	rBV	1578425	1372259	36.06%	4.406%
7	9.372	1106	1111	1114	rBV	4192000	3709475	97.47%	11.911%
8	10.054	1223	1227	1231	rVB	1968754	1608239	42.26%	5.164%
9	10.230	1254	1257	1265	rBV6	34406	67598	1.78%	0.217%
10	10.766	1345	1348	1352	rVB	355809	308523	8.11%	0.991%
11	10.848	1358	1362	1366	rBV	2841386	2533941	66.58%	8.136%
12	11.548	1477	1481	1485	rBV	1912806	1777715	46.71%	5.708%
13	11.648	1495	1498	1502	rVB	87755	77921	2.05%	0.250%
14	12.060	1553	1568	1574	rBV	587383	812468	21.35%	2.609%
15	12.213	1591	1594	1596	rBV	82880	80142	2.11%	0.257%
16	12.248	1597	1600	1608	rVB2	88797	149879	3.94%	0.481%
17	12.313	1608	1611	1615	rVB	81643	70118	1.84%	0.225%
18	12.771	1683	1689	1693	rBV	71475	96667	2.54%	0.310%
19	12.848	1697	1702	1715	rVV2	173216	279980	7.36%	0.899%
20	13.001	1725	1728	1730	rBV	55348	46100	1.21%	0.148%
21	13.083	1738	1742	1748	rVB2	55492	88990	2.34%	0.286%
22	13.142	1748	1752	1755	rBV	4318687	3805850	100.00%	12.220%
23	13.701	1842	1847	1849	rVB3	37071	44051	1.16%	0.141%
24	13.818	1862	1867	1874	rVB2	92456	172081	4.52%	0.553%
25	14.036	1900	1904	1919	rBV	162624	310793	8.17%	0.998%
26	14.207	1929	1933	1936	rBV	1340743	1178909	30.98%	3.785%
27	14.401	1962	1966	1976	rBV	86941	140653	3.70%	0.452%
28	14.942	2053	2058	2062	rBV	73517	115610	3.04%	0.371%
29	15.348	2125	2127	2136	rVB6	30779	45198	1.19%	0.145%
30	15.536	2155	2159	2167	rVB2	58571	107085	2.81%	0.344%
31	15.759	2192	2197	2203	rVB	751561	957236	25.15%	3.074%

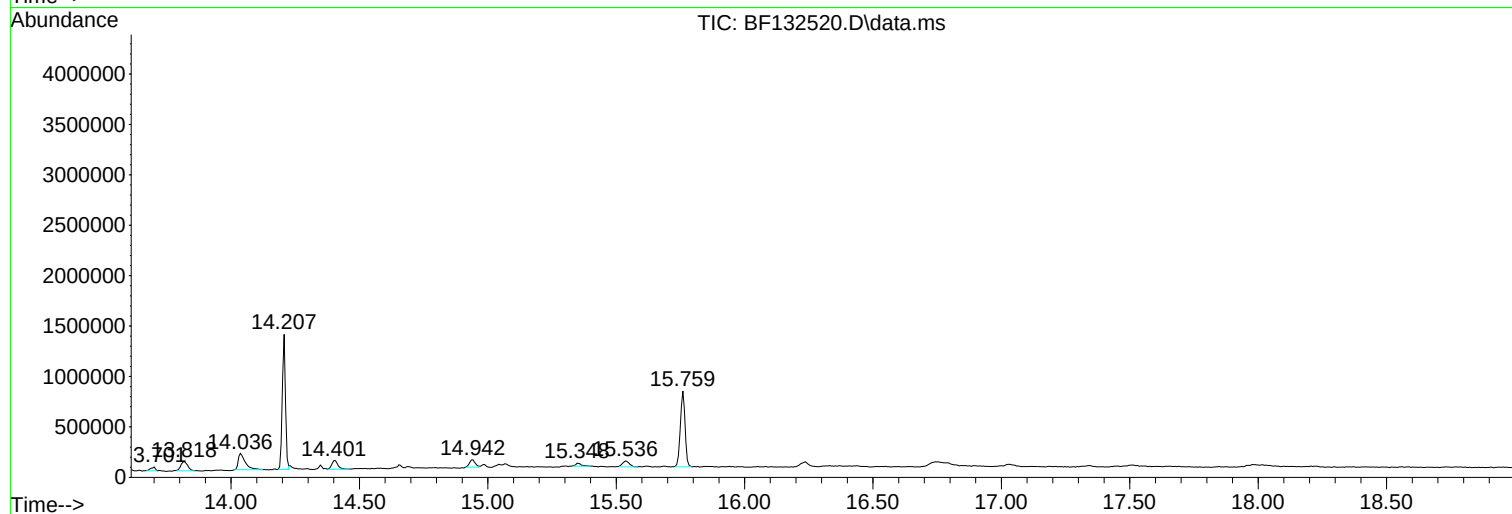
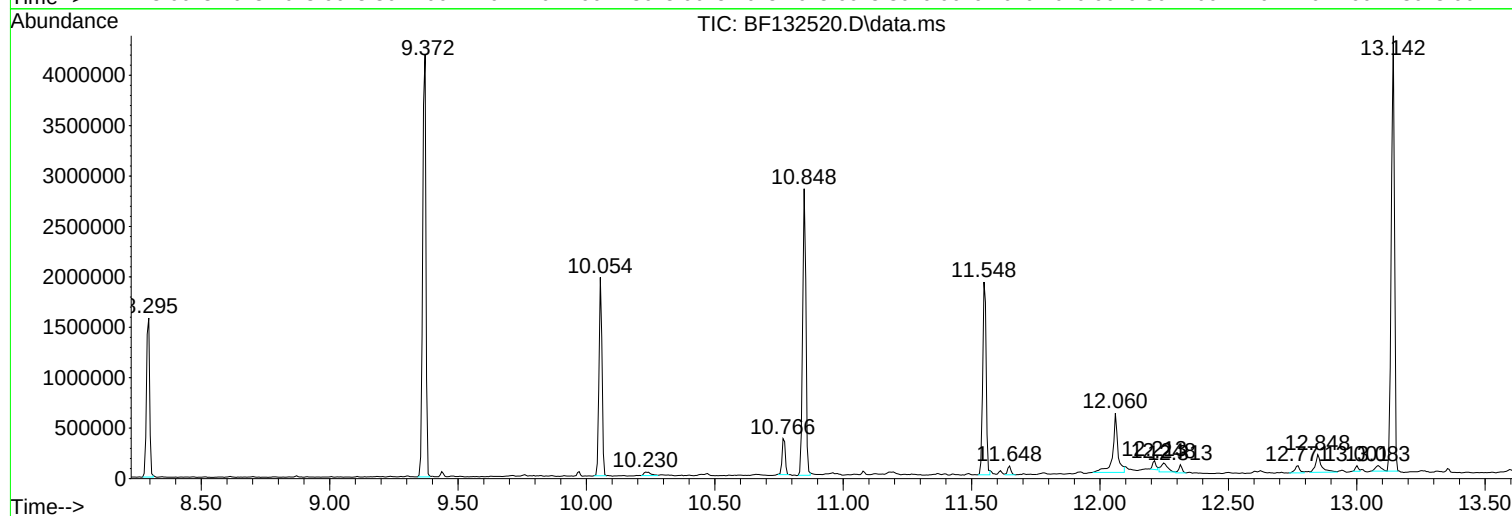
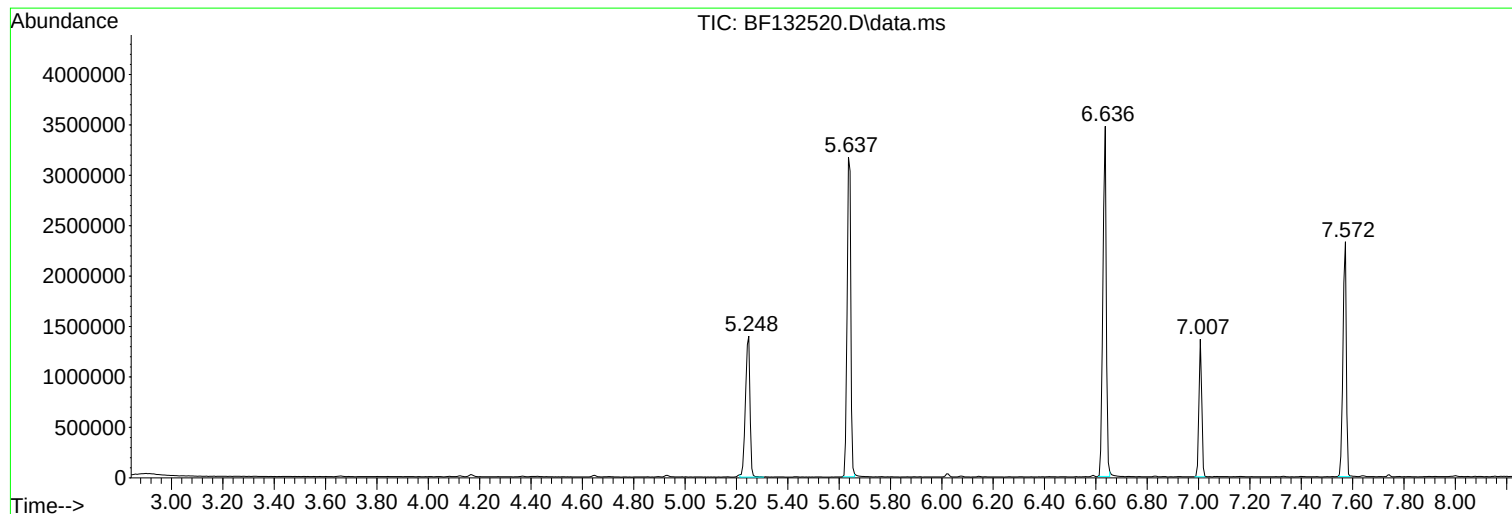
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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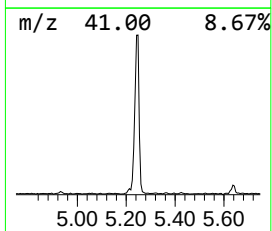
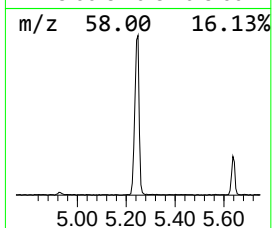
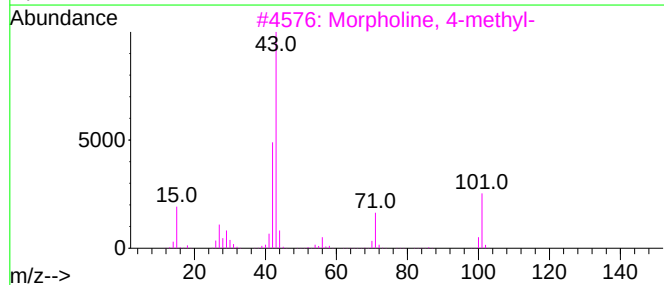
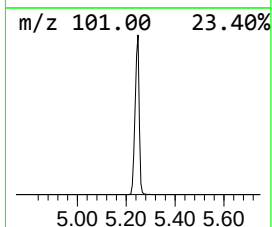
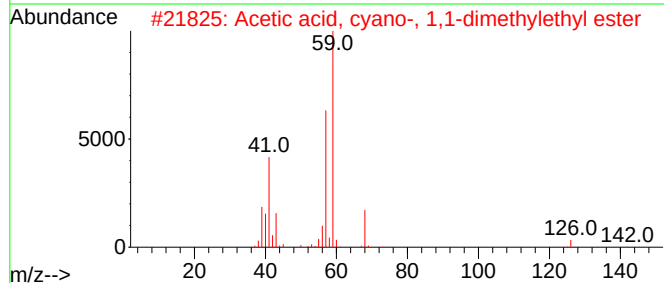
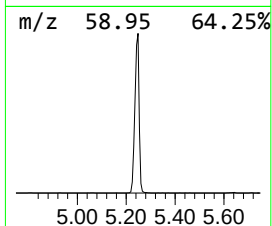
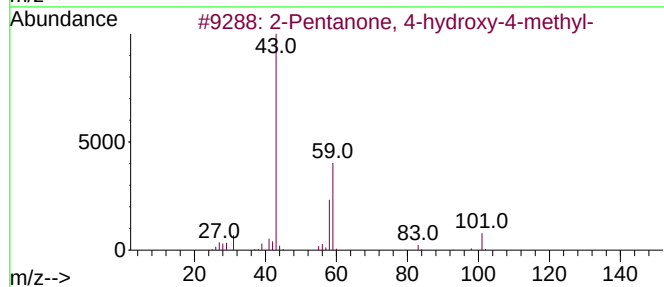
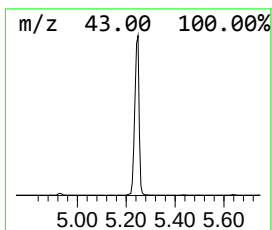
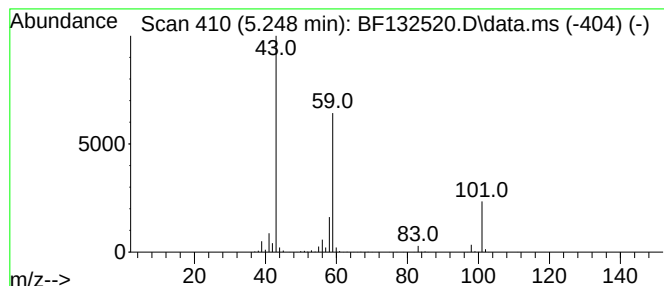
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.248	31.89 ng	1686900	1,4-Dichlorobenzene-d4	7.007

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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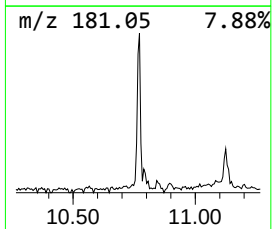
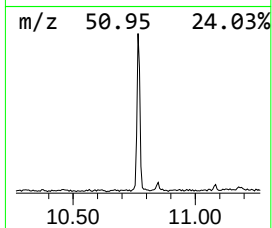
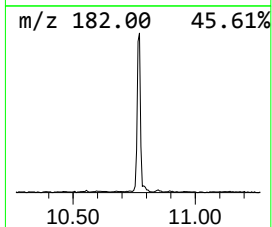
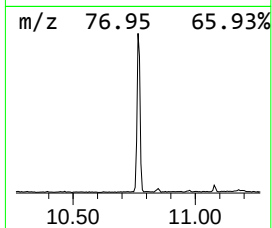
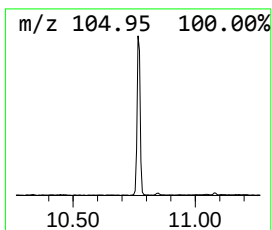
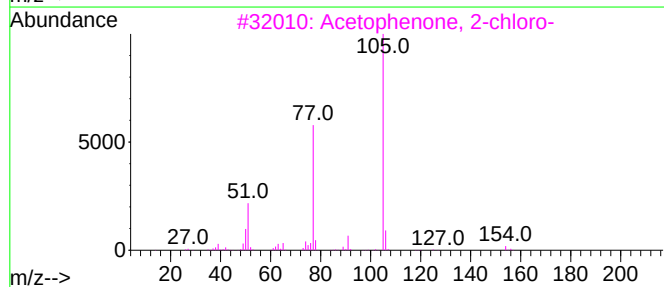
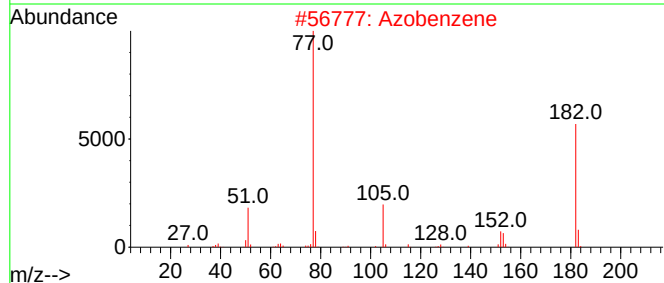
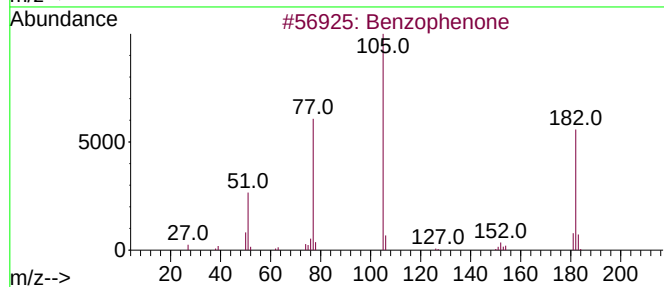
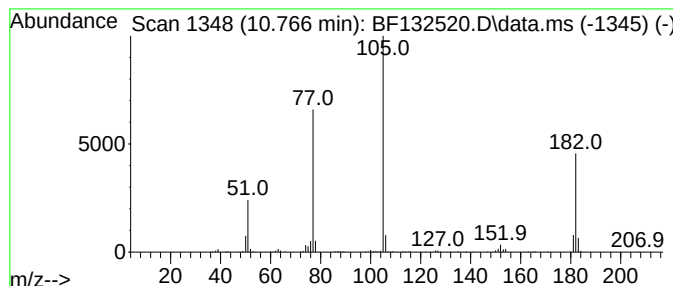
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.766	3.84 ng	308523	Acenaphthene-d10	10.054

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	53
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



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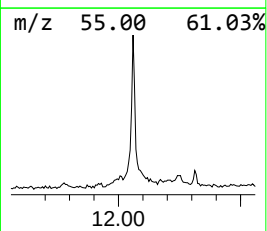
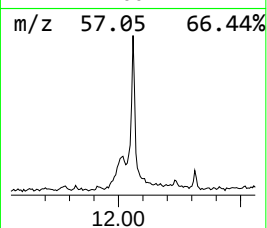
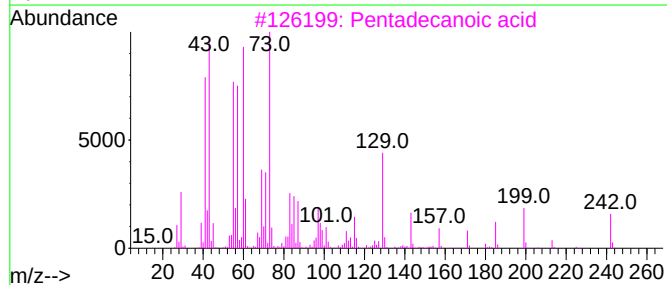
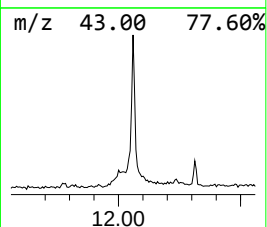
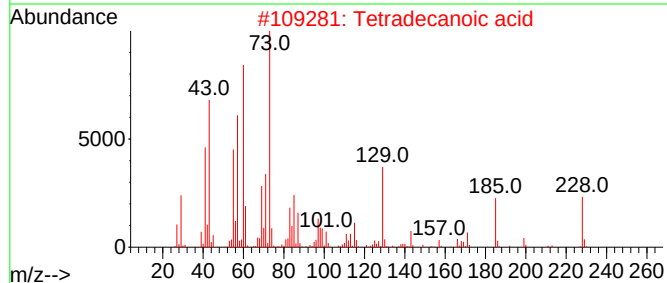
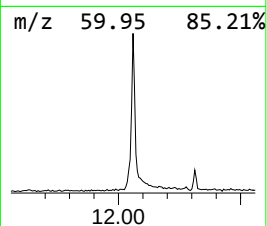
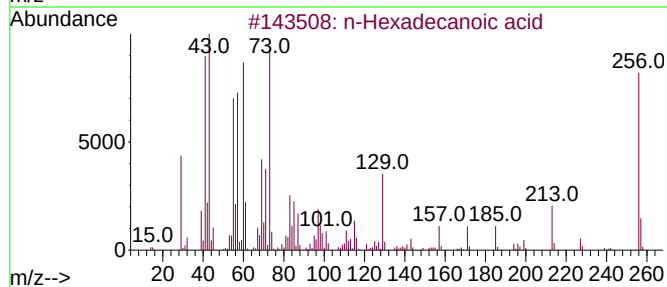
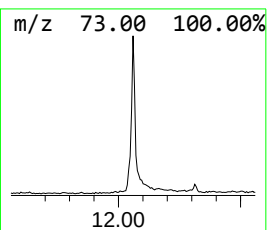
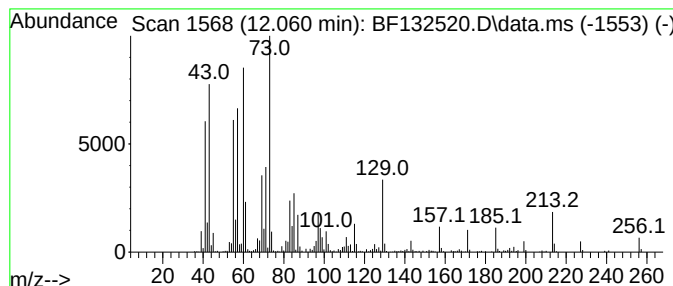
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	9.14 ng	812468	Phenanthrene-d10	11.548

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			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	87
5			Nonanoic acid	158	C9H18O2	000112-05-0	43



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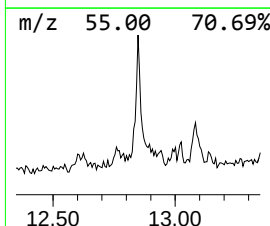
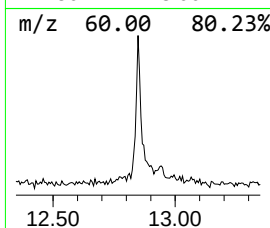
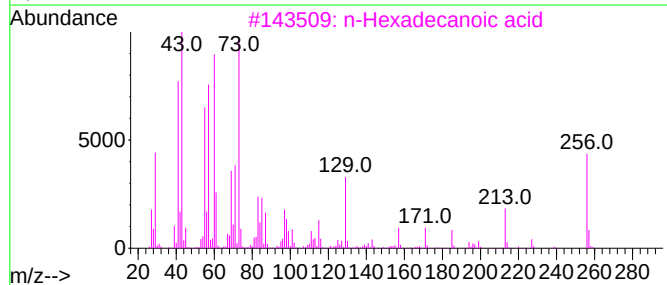
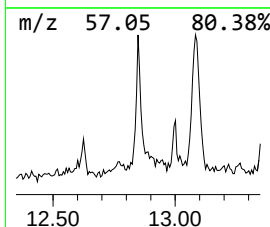
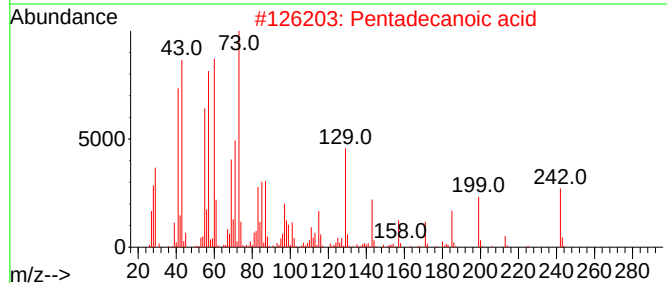
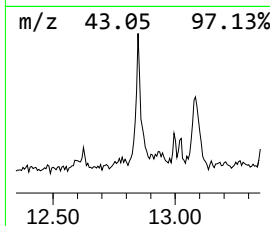
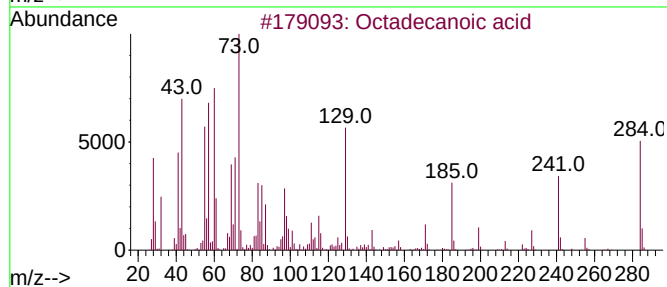
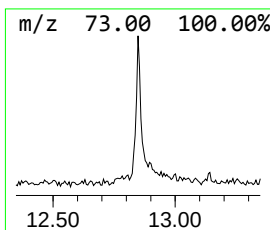
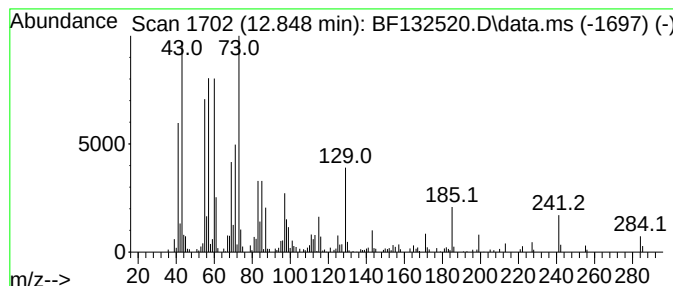
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.848	3.15 ng	279980	Phenanthrene-d10	11.548

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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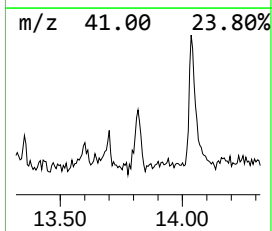
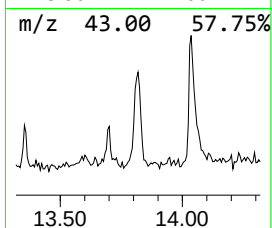
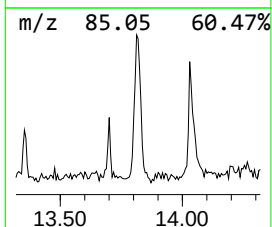
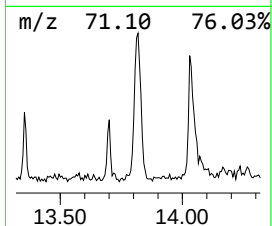
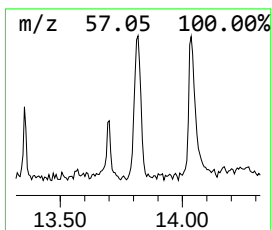
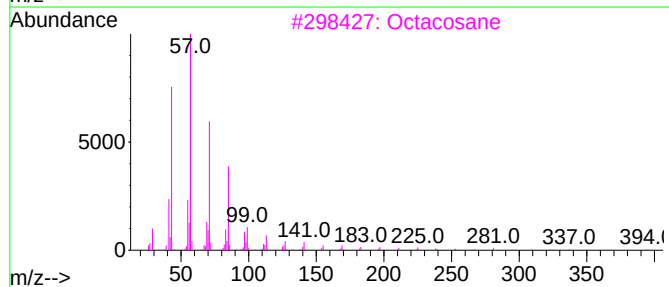
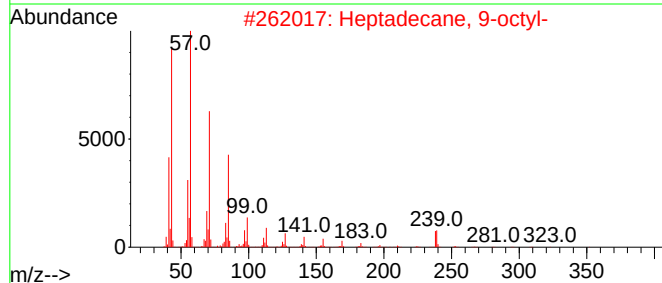
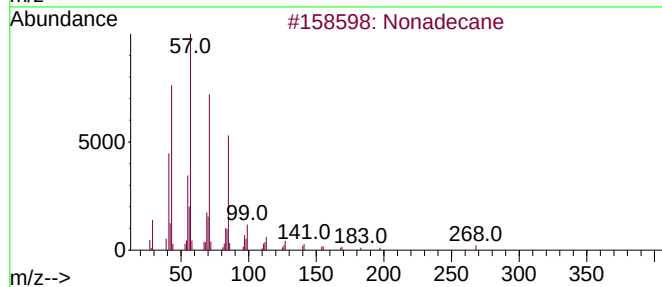
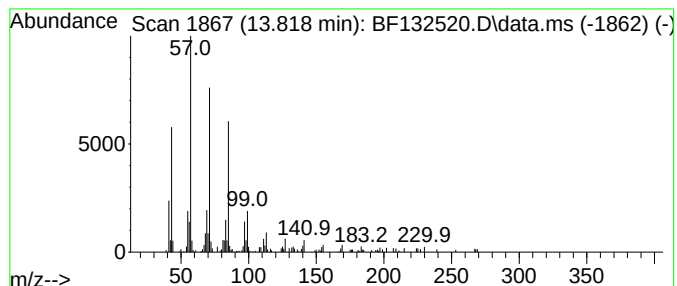
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.818	2.92 ng	172081	Chrysene-d12	14.207

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



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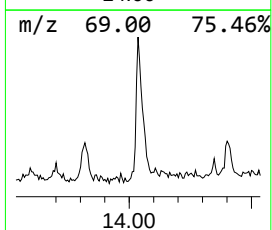
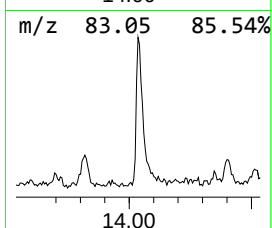
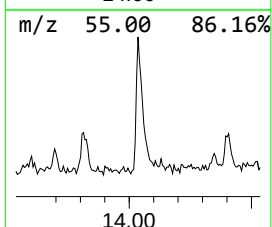
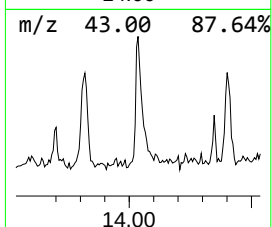
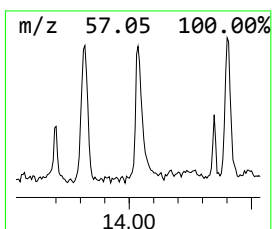
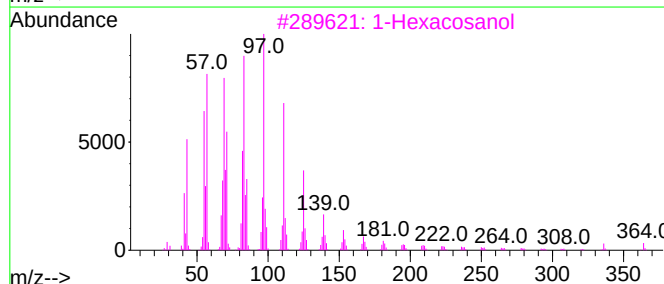
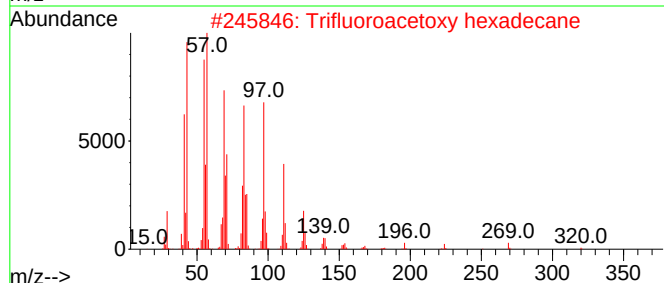
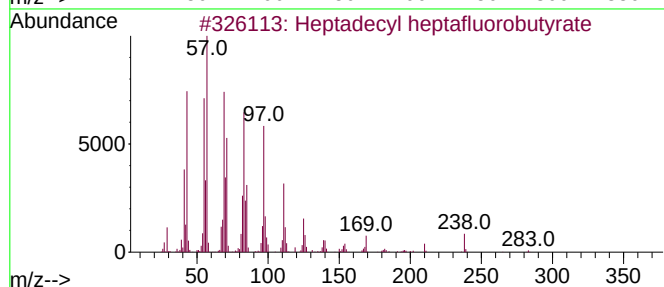
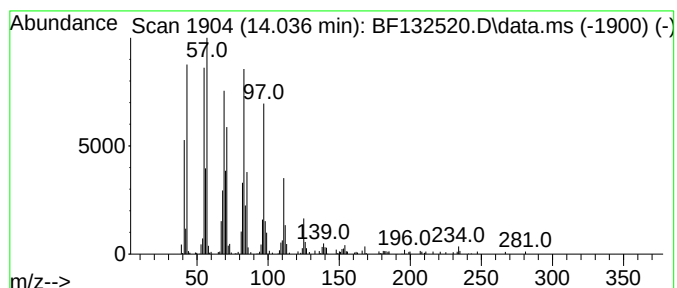
Instrument :
BNA_F
ClientSampleId :
B-17-SB01

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 6 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.036	5.27 ng	310793	Chrysene-d12	14.207	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	1-Hexacosanol	382	C26H54O	000506-52-5	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	1-Hexacosene	364	C26H52	018835-33-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022323\
Data File : BF132520.D
Acq On : 23 Feb 2023 14:58
Operator : CG\JU
Sample : 01657-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-17-SB01

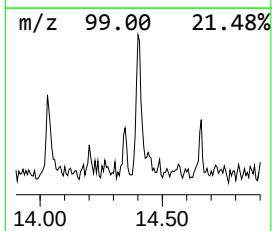
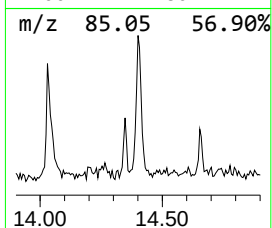
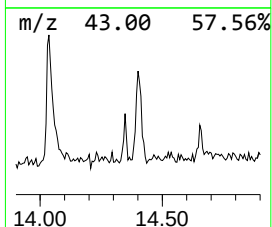
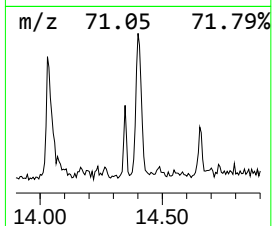
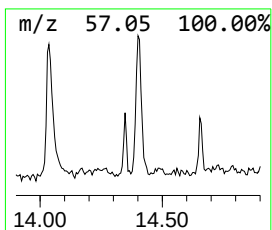
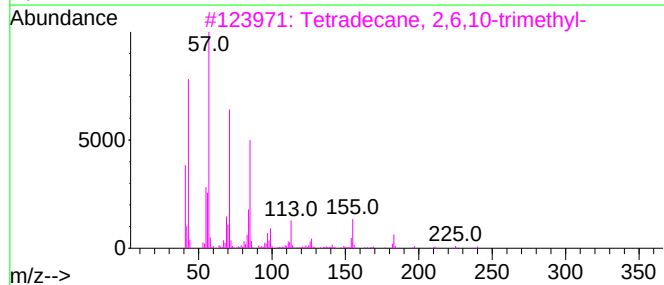
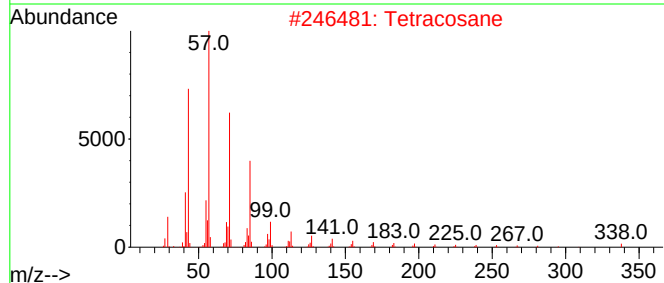
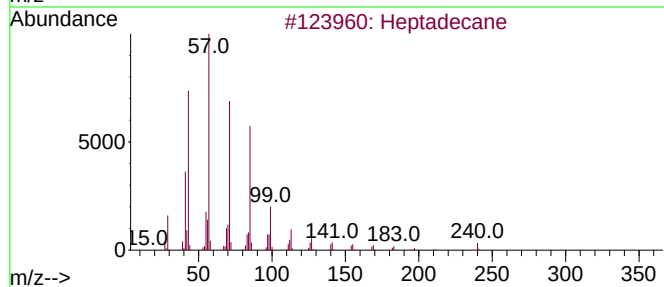
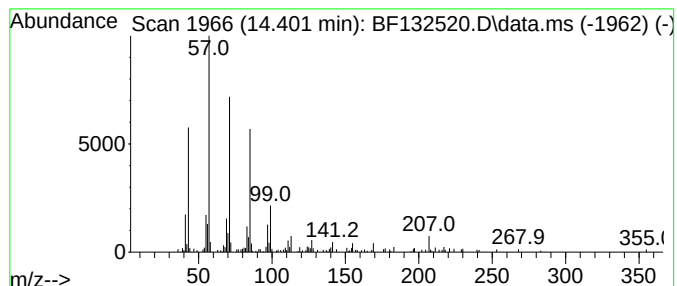
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.401	2.39 ng	140653	Chrysene-d12	14.207

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	93
2			Tetracosane	338	C24H50	000646-31-1	80
3			Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	80
4			Nonadecane	268	C19H40	000629-92-5	74
5			Docosane	310	C22H46	000629-97-0	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022323\
Data File : BF132520.D
Acq On : 23 Feb 2023 14:58
Operator : CG\JU
Sample : 01657-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-17-SB01

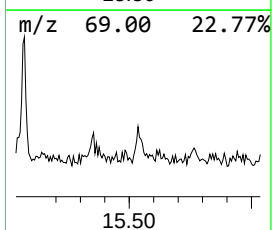
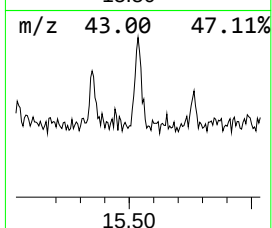
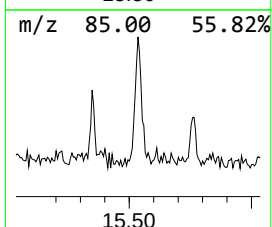
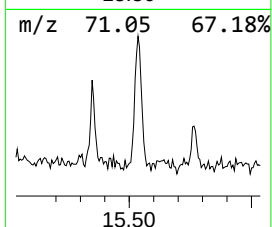
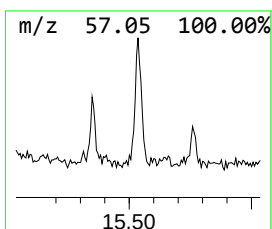
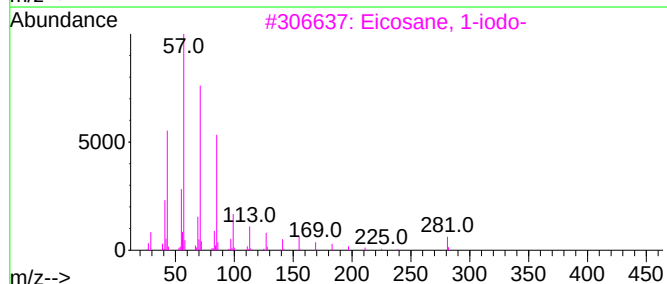
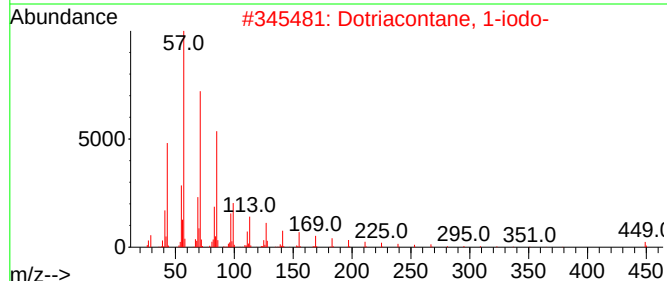
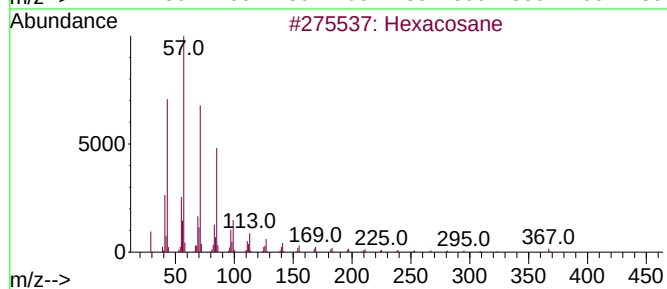
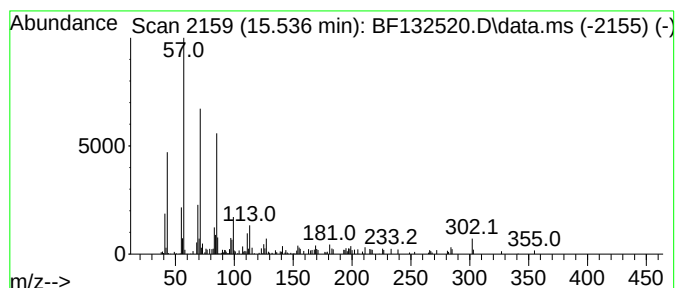
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.536	2.24 ng	107085	Perylene-d12	15.759

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	86
2			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	86
3			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	83
4			5,5-Diethylheptadecane	296	C21H44	1010360-41-7	80
5			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022323\
Data File : BF132520.D
Acq On : 23 Feb 2023 14:58
Operator : CG\JU
Sample : 01657-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-17-SB01

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-...	5.248	31.9	ng	1686900	1	7.007	1057790	20.0
Benzophenone	10.766	3.8	ng	308523	3	10.054	1608240	20.0
n-Hexadecanoic ...	12.060	9.1	ng	812468	4	11.548	1777720	20.0
Octadecanoic acid	12.848	3.1	ng	279980	4	11.548	1777720	20.0
Nonadecane	13.818	2.9	ng	172081	5	14.207	1178910	20.0
Heptadecyl hept...	14.036	5.3	ng	310793	5	14.207	1178910	20.0
Heptadecane	14.401	2.4	ng	140653	5	14.207	1178910	20.0
Hexacosane	15.536	2.2	ng	107085	6	15.759	957236	20.0