LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
Data File : BF139721.D
Acq On : 09 Oct 2024 14:36
Operator : RC/JU
Sample : P4340-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1B-3

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-BF100124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139721.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.158	3	11	18	rBV	2171199	3577708	100.00%	16.504%
2	5.087	498	509	521	rVB	106889	177208	4.95%	0.817%
3	5.487	571	577	593	rBV	1606656	2174379	60.78%	10.031%
4	6.498	737	749	772	rBV	1661341	2275314	63.60%	10.496%
5	6.863	806	811	816	rBV	430798	517088	14.45%	2.385%
6	7.428	901	907	912	rBV	1120808	1467428	41.02%	6.769%
7	7.681	945	950	955	rBV	52101	64904	1.81%	0.299%
8	8.145	1023	1029	1034	rBV	547389	672271	18.79%	3.101%
9	8.363	1061	1066	1076	rVB2	27521	37389	1.05%	0.172%
10	9.222	1206	1212	1217	rBV	2002532	2522923	70.52%	11.639%
11	9.898	1322	1327	1332	rBV	627829	762789	21.32%	3.519%
12	10.616	1443	1449	1456	rVB	441388	573154	16.02%	2.644%
13	10.692	1456	1462	1474	rBV	1150203	1557561	43.54%	7.185%
14	10.922	1496	1501	1509	rVB	51520	68179	1.91%	0.315%
15	11.386	1575	1580	1585	rBV	658383	810189	22.65%	3.738%
16	11.910	1664	1669	1691	rBV2	261607	465853	13.02%	2.149%
17	12.692	1798	1802	1814	rVV	47317	90664	2.53%	0.418%
18	12.975	1844	1850	1855	rBV	1726354	2294972	64.15%	10.587%
19	13.445	1923	1930	1937	rBV	158575	243013	6.79%	1.121%
20	13.874	1997	2003	2020	rBV3	56586	153197	4.28%	0.707%
21	14.027	2020	2029	2034	rBV	392423	558940	15.62%	2.578%
22	14.186	2052	2056	2068	rVB	24291	42832	1.20%	0.198%
23	14.486	2103	2107	2112	rBV	28496	37410	1.05%	0.173%
24	14.798	2155	2160	2164	rBV	27630	41444	1.16%	0.191%
25	15.133	2213	2217	2223	rVB	27822	39907	1.12%	0.184%
26	15.498	2273	2279	2289	rBV	279284	450562	12.59%	2.078%

Sum of corrected areas: 21677278

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Instrument :
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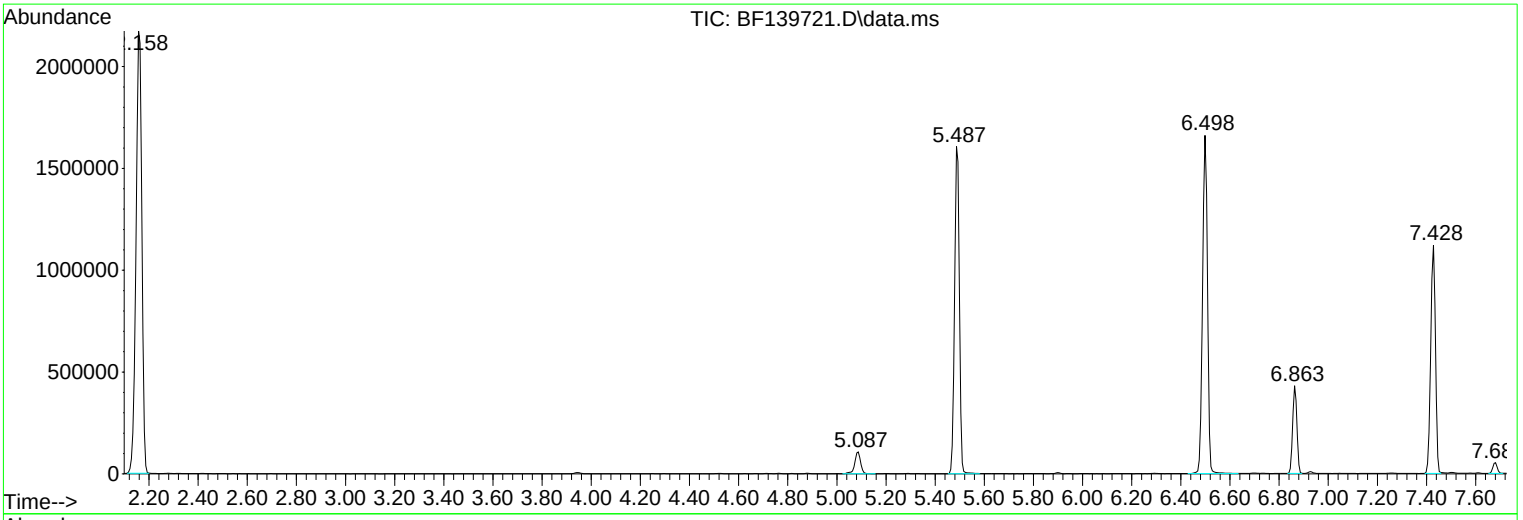
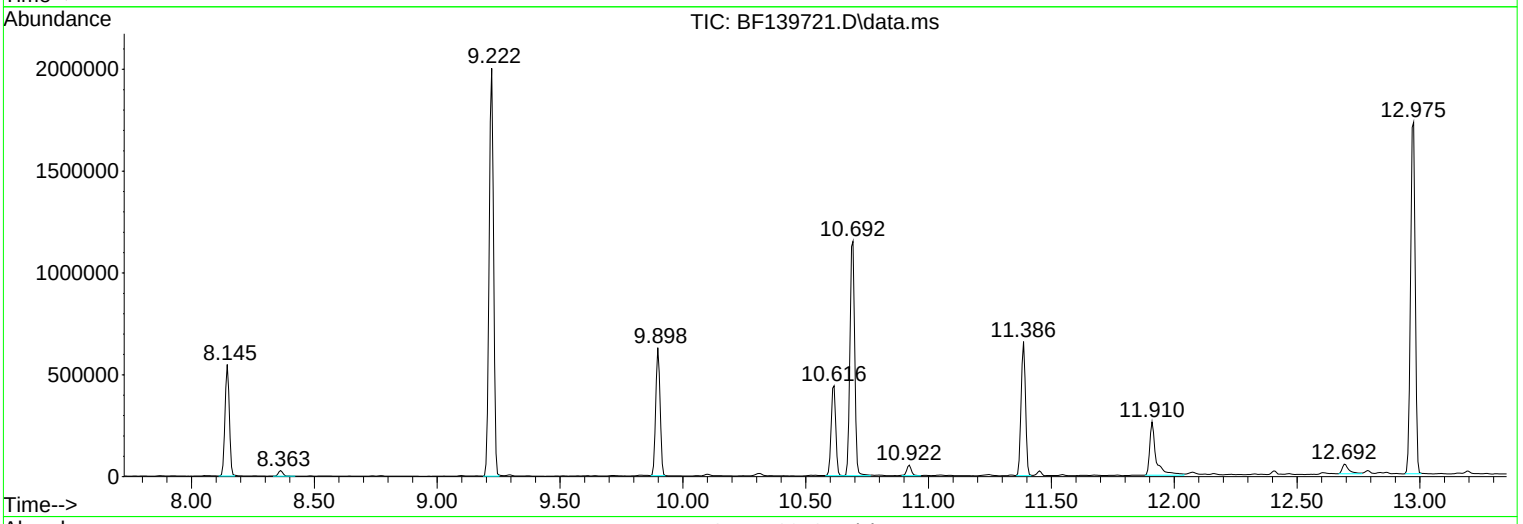
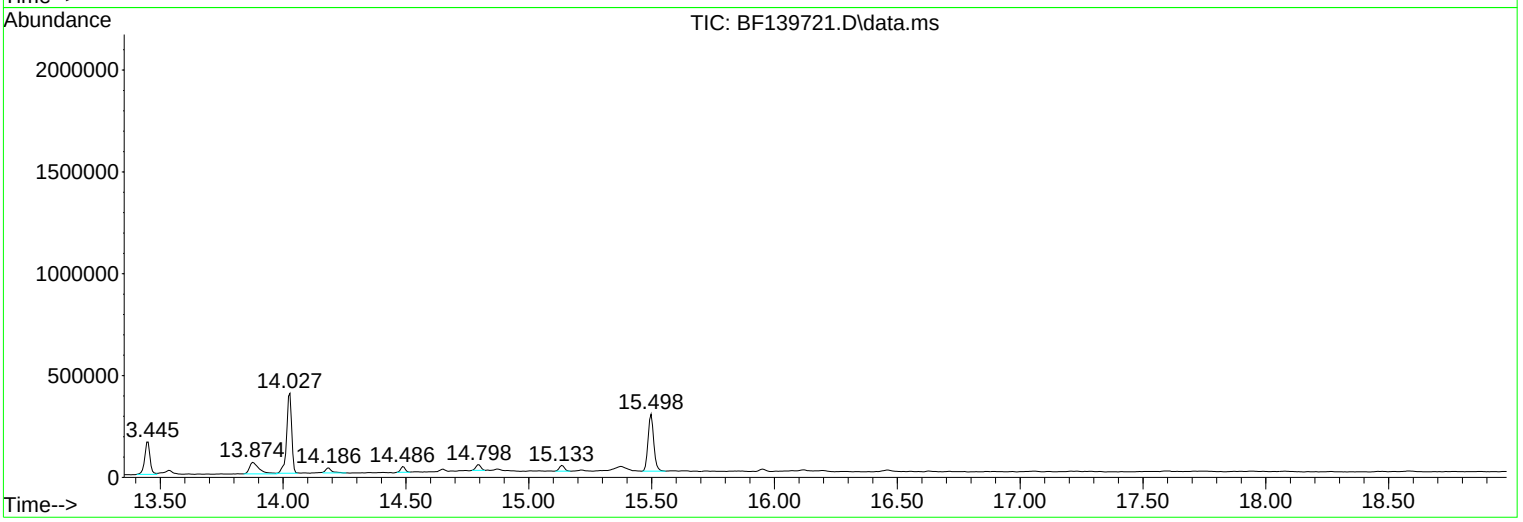
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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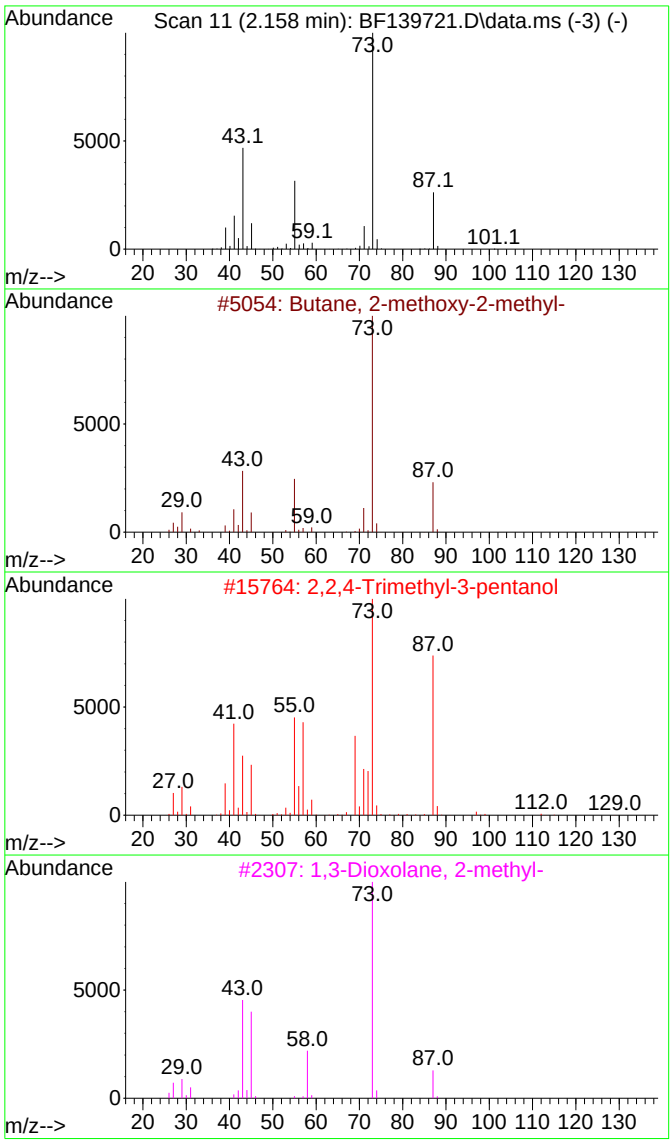
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

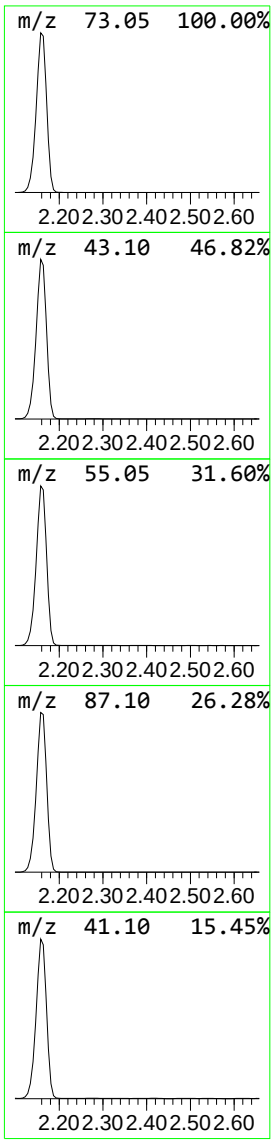
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.158	138.38 ng	3577710	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Acq On : 09 Oct 2024 14:36
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Sample : P4340-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1B-3

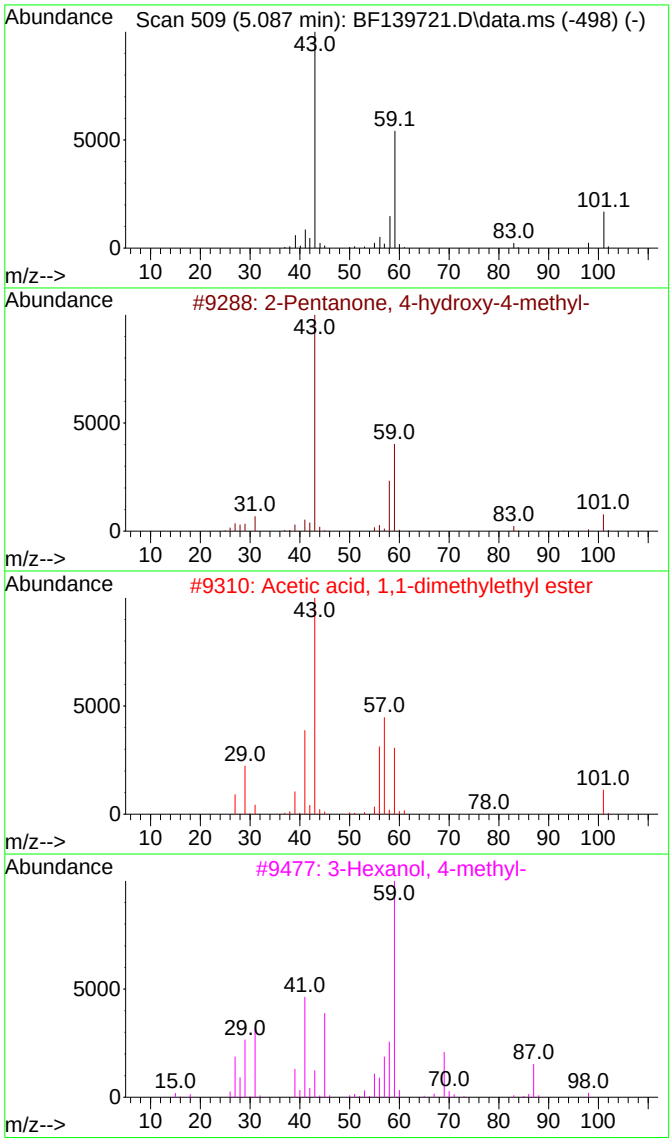
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

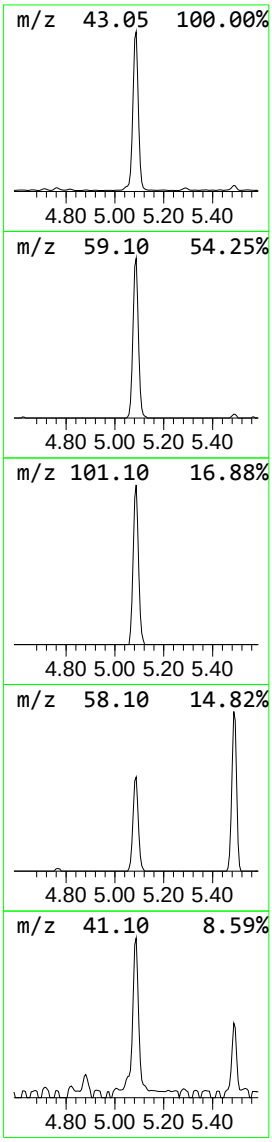
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	6.85 ng	177208	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
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Acq On : 09 Oct 2024 14:36
Operator : RC/JU
Sample : P4340-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

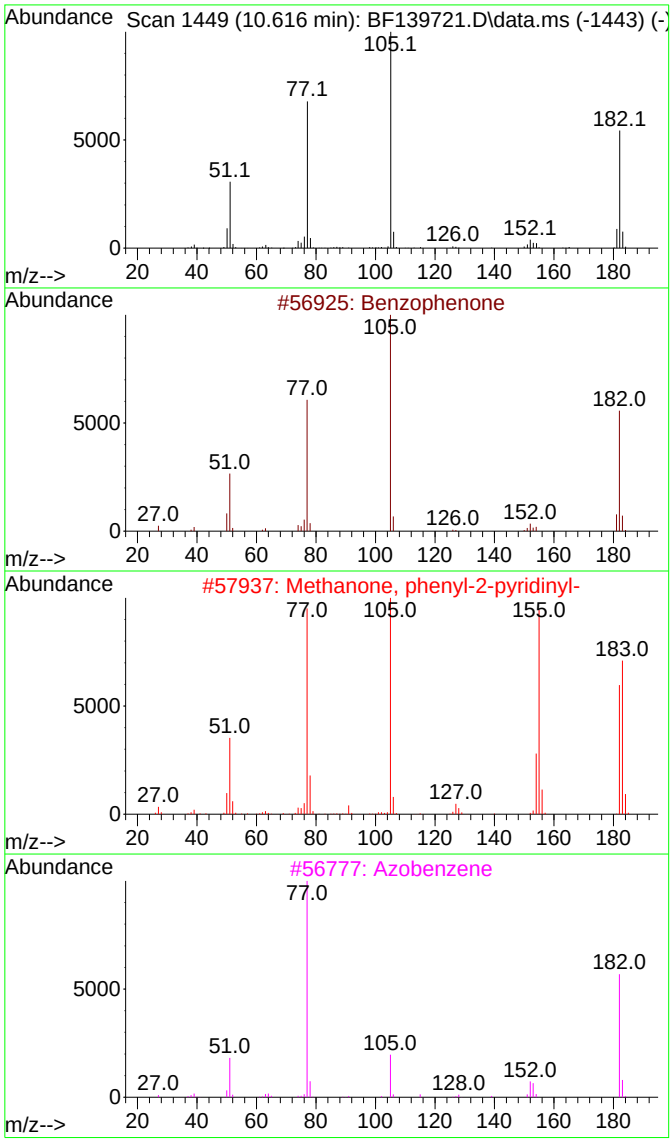
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

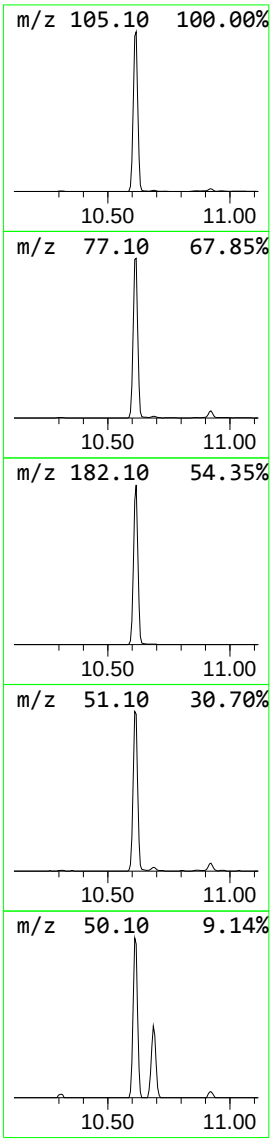
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	15.03 ng	573154	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	78
3	Azobenzene	182	C12H10N2	000103-33-3	58
4	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	50
5	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50





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Sample : P4340-05
Misc :
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Instrument :
BNA_F
ClientSampleId :
1B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

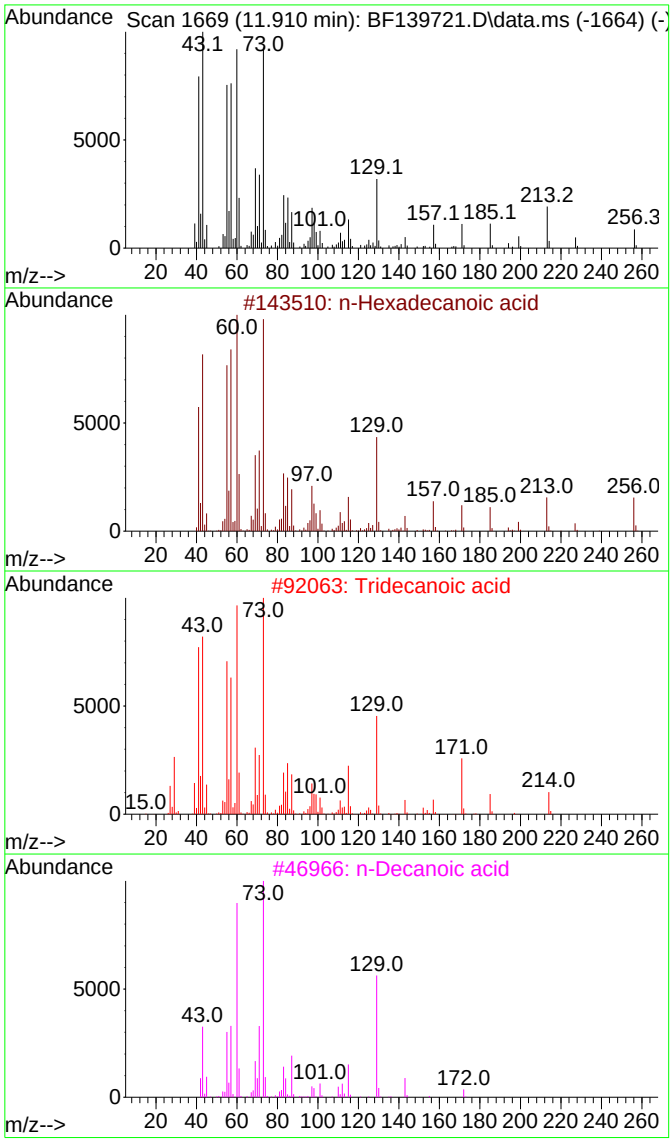
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

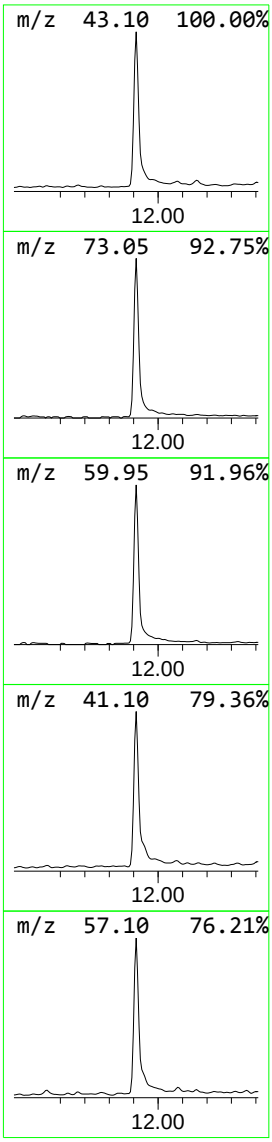
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	11.50 ng	465853	Phenanthrene-d10	11.386

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	94
3	n-Decanoic acid	172	C10H20O2	000334-48-5	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100924\
Data File : BF139721.D
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Operator : RC/JU
Sample : P4340-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1B-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

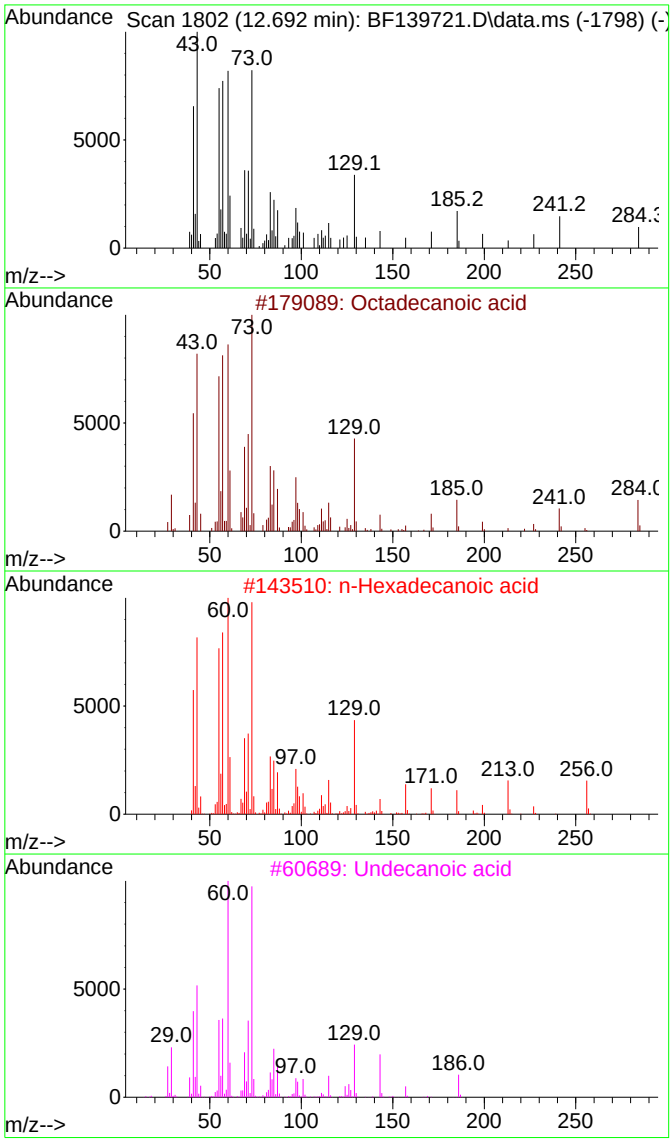
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

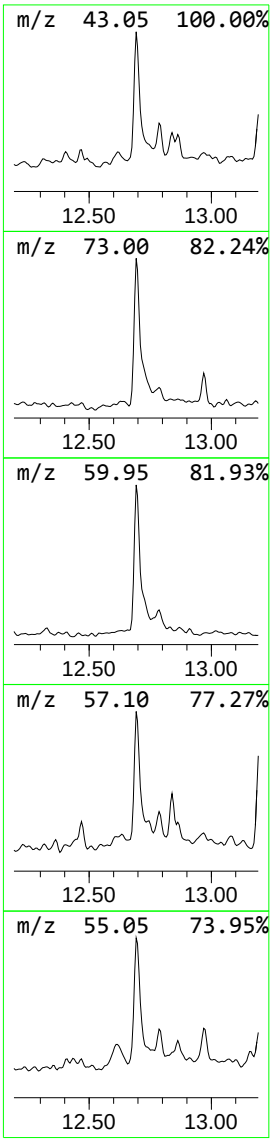
****

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.692	2.24 ng	90664	Phenanthrene-d10	11.386

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	83
3	Undecanoic acid	186	C11H22O2	000112-37-8	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72





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BNA_F
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TIC Library : C:\Database\NIST20.L
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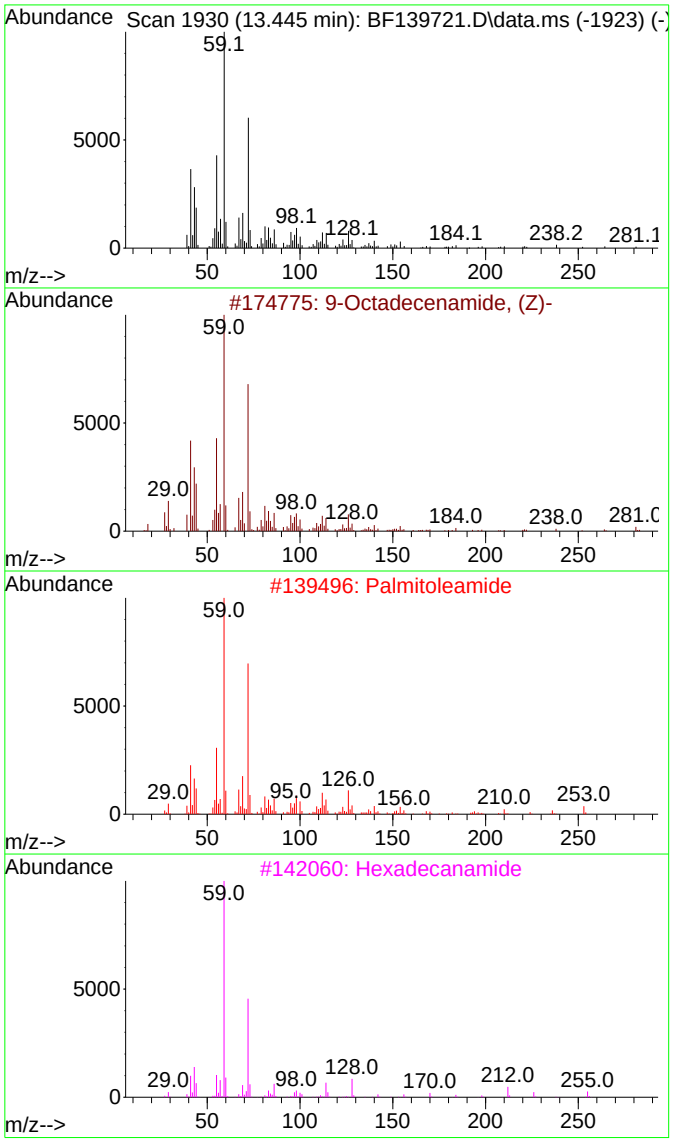
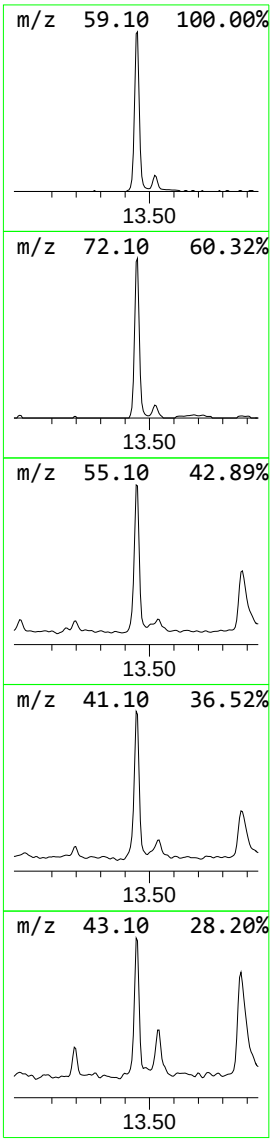
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.445	8.70 ng	243013	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Palmitoleamide	253	C16H31NO	106010-22-4	86
3	Hexadecanamide	255	C16H33NO	000629-54-9	72
4	Octadecanamide	283	C18H37NO	000124-26-5	53
5	Octanamide	143	C8H17NO	000629-01-6	53





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BNA_F
ClientSampleId :
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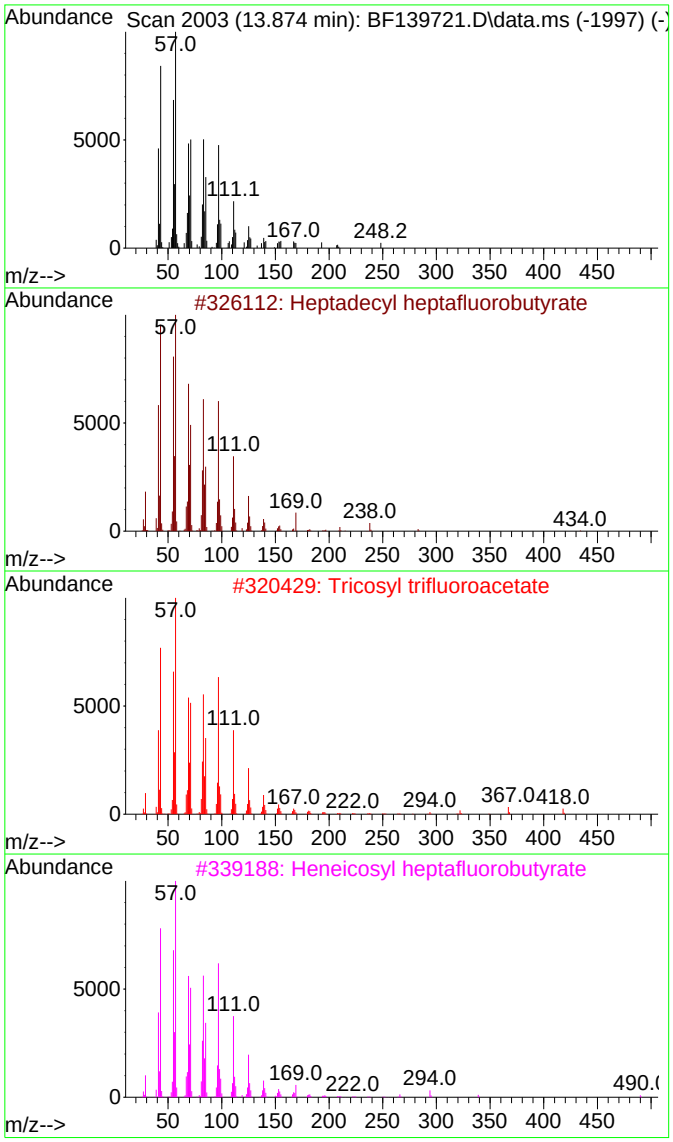
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

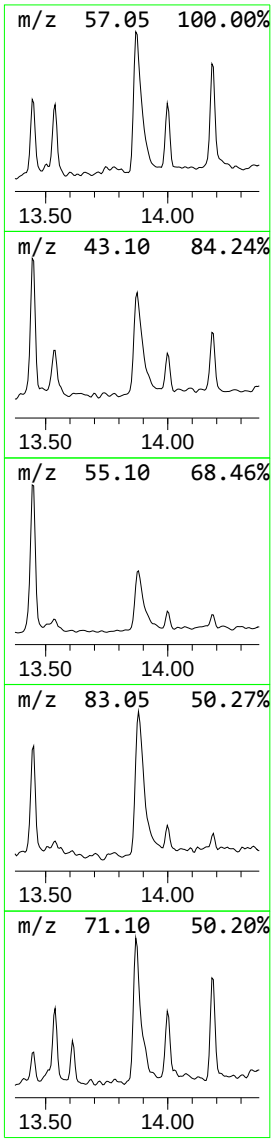
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.48 ng	153197	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
4	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
5	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1010351-81-4	91





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.158	138.4	ng	3577710	1	6.863	517088	20.0
2-Pentanone, 4-...	5.087	6.8	ng	177208	1	6.863	517088	20.0
Benzophenone	10.616	15.0	ng	573154	3	9.898	762789	20.0
n-Hexadecanoic ...	11.910	11.5	ng	465853	4	11.386	810189	20.0
Octadecanoic acid	12.692	2.2	ng	90664	4	11.386	810189	20.0
9-Octadecenamid...	13.445	8.7	ng	243013	5	14.027	558940	20.0
Heptadecyl hept...	13.874	5.5	ng	153197	5	14.027	558940	20.0