LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111424\
Data File : BF140383.D
Acq On : 15 Nov 2024 00:32
Operator : RC/JU
Sample : P4807-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BF-F14

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-BF111324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140383.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	3	10	20	rVB	900754	1387372	51.13%	6.982%
2	5.098	500	511	520	rVB	46027	74303	2.74%	0.374%
3	5.516	576	582	595	rBV	1923537	2532992	93.36%	12.747%
4	6.528	748	754	774	rVB	1960876	2640833	97.33%	13.289%
5	6.875	808	813	819	rBV	581874	733498	27.03%	3.691%
6	7.439	903	909	914	rBV	1227491	1586783	58.48%	7.985%
7	7.686	944	951	957	rBV	65023	82036	3.02%	0.413%
8	8.157	1026	1031	1043	rBV	723000	891048	32.84%	4.484%
9	8.369	1063	1067	1077	rBV	22326	31453	1.16%	0.158%
10	9.233	1208	1214	1223	rBV	2071295	2713261	100.00%	13.654%
11	9.910	1324	1329	1341	rBV	644040	830225	30.60%	4.178%
12	10.622	1445	1450	1459	rBV	209177	274118	10.10%	1.379%
13	10.704	1459	1464	1474	rBV	1043975	1343000	49.50%	6.758%
14	11.404	1577	1583	1589	rBV	580754	745710	27.48%	3.753%
15	11.921	1666	1671	1684	rBV2	176027	327223	12.06%	1.647%
16	12.633	1786	1792	1801	rBV	130767	350856	12.93%	1.766%
17	12.710	1802	1805	1817	rVB2	46578	101055	3.72%	0.509%
18	12.986	1847	1852	1858	rBV	1713957	2202326	81.17%	11.083%
19	13.892	2002	2006	2015	rVB2	81095	154480	5.69%	0.777%
20	14.045	2028	2032	2037	rVB	401724	517605	19.08%	2.605%
21	15.533	2281	2285	2294	rVB	235659	351523	12.96%	1.769%

Sum of corrected areas: 19871700

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111424\
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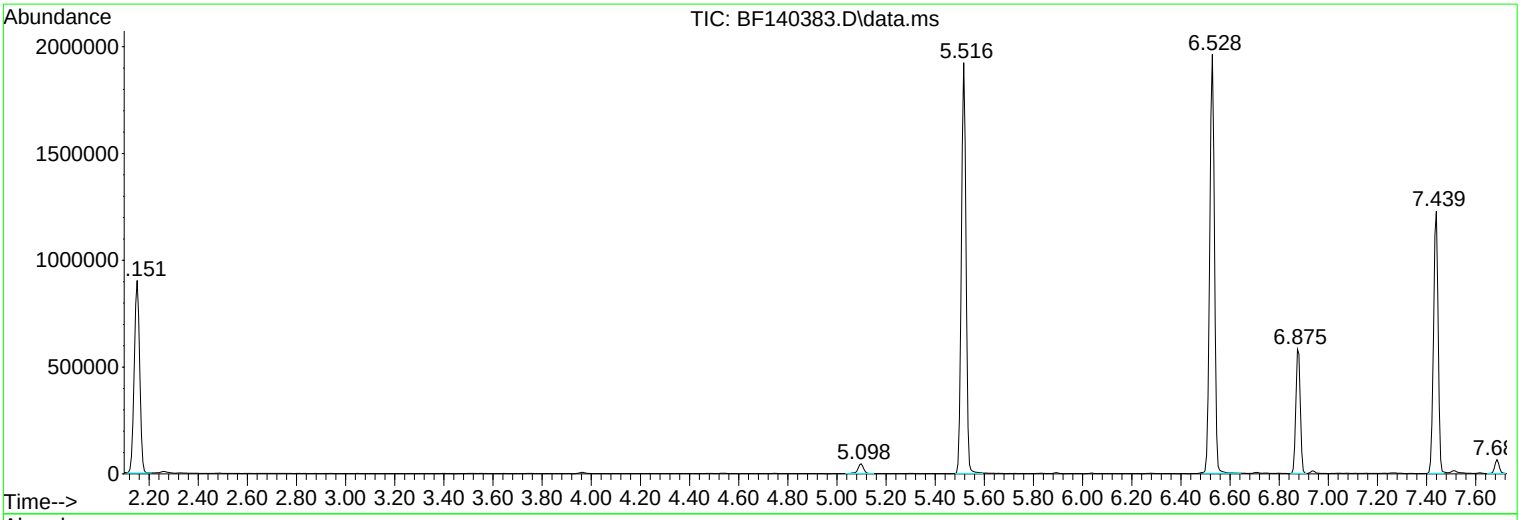
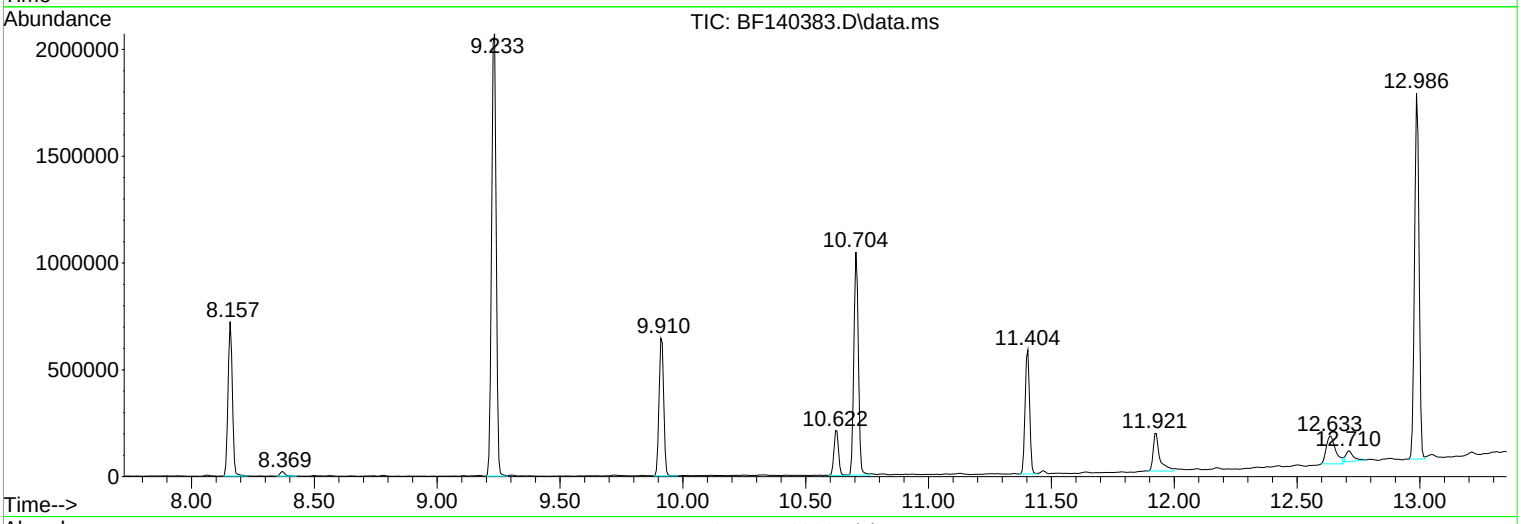
Misc :
ALS Vial : 19 Sample Multiplier: 1

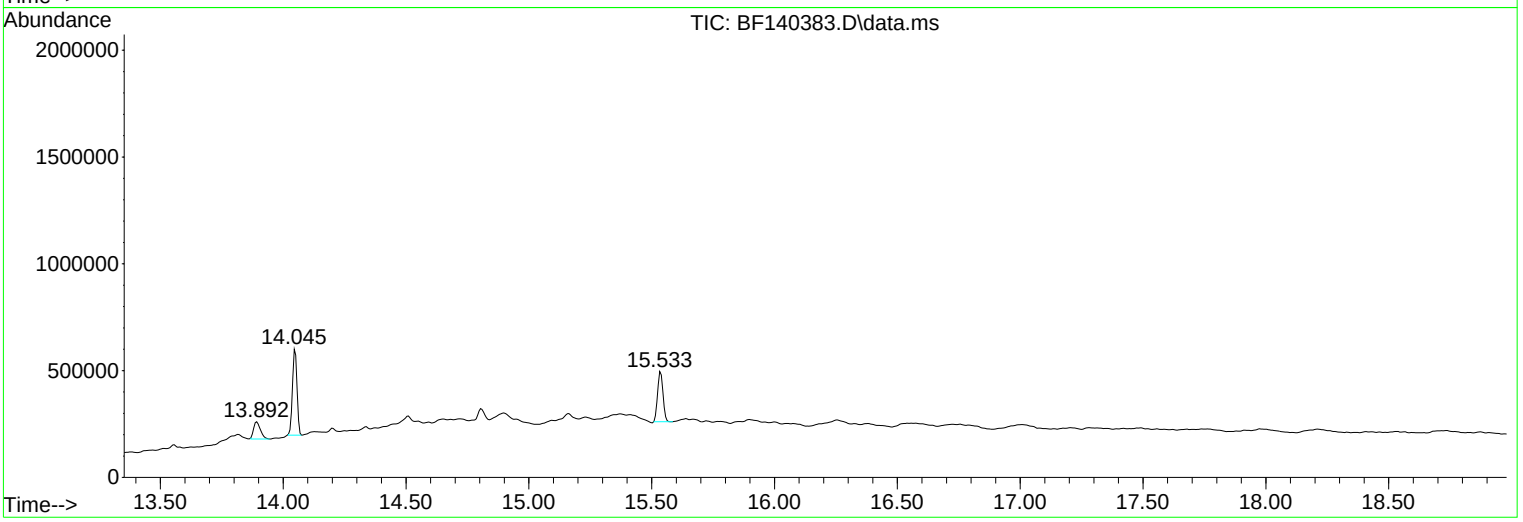
Instrument :
BNA_F
ClientSampleId :
BF-F14

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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

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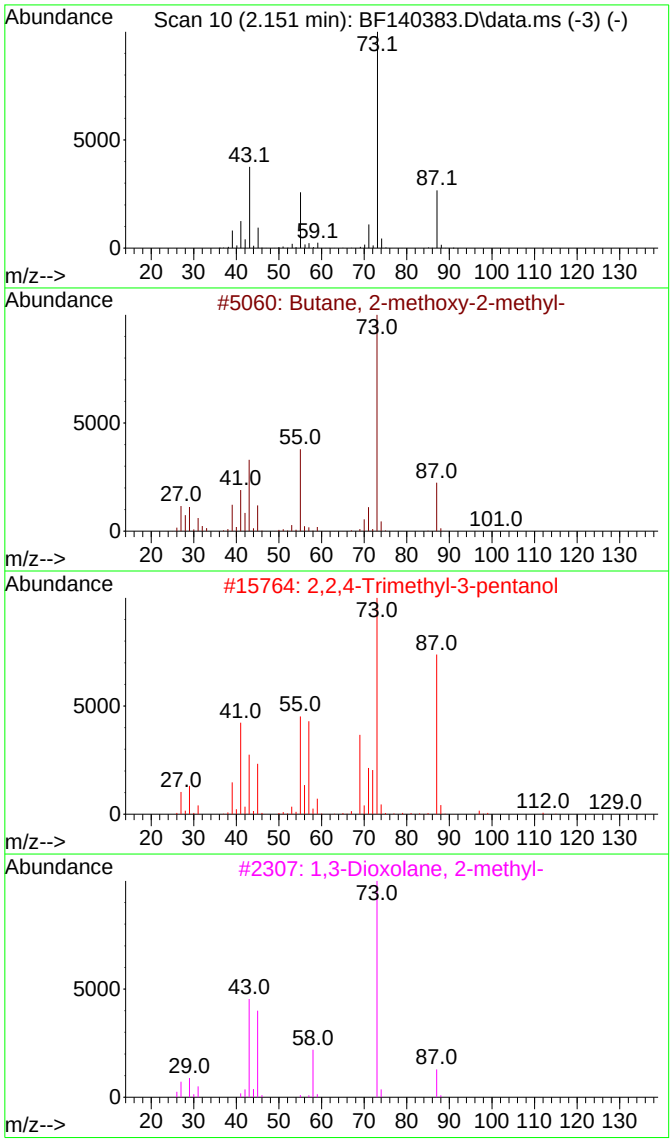
TIC Integration Parameters: LSCINT.P

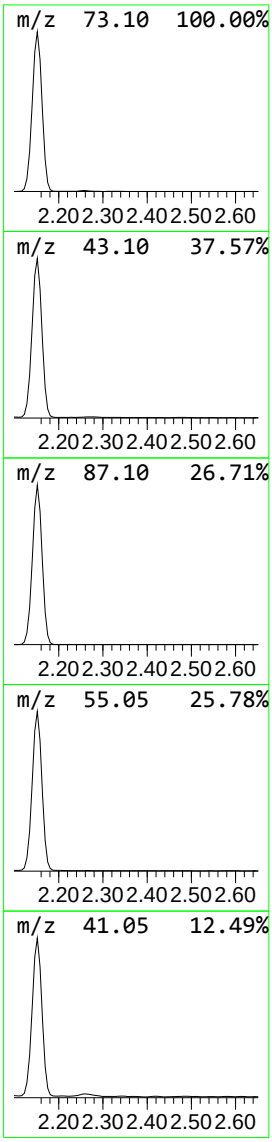
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.151	37.83 ng	1387370	1,4-Dichlorobenzene-d4	6.875

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	25
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Data File : BF140383.D
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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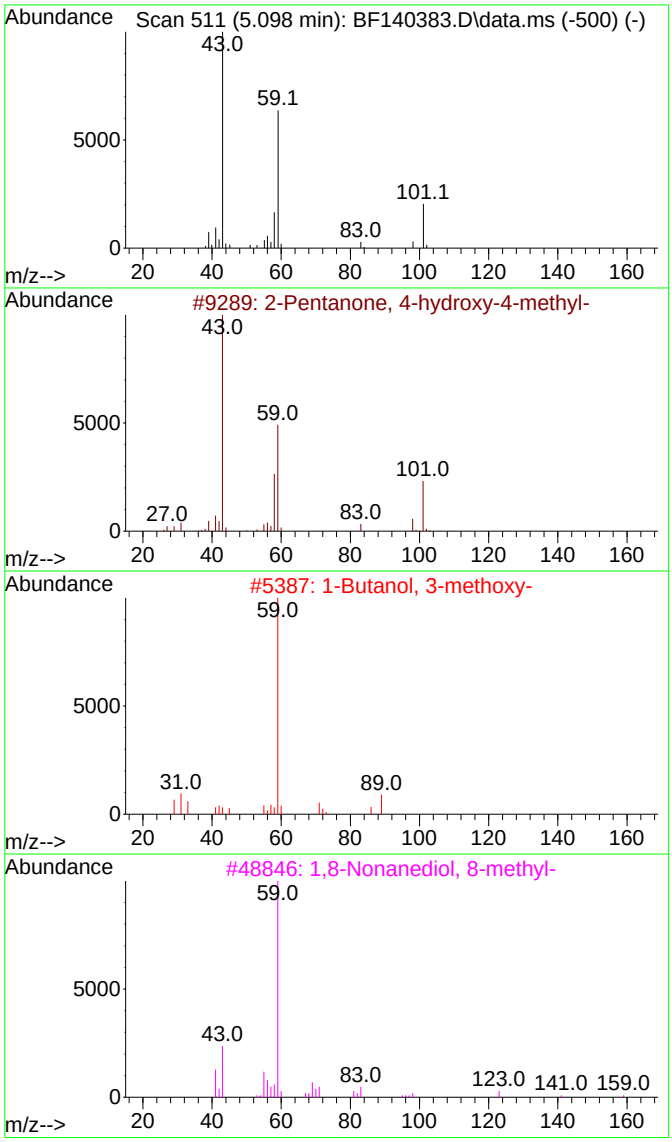
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

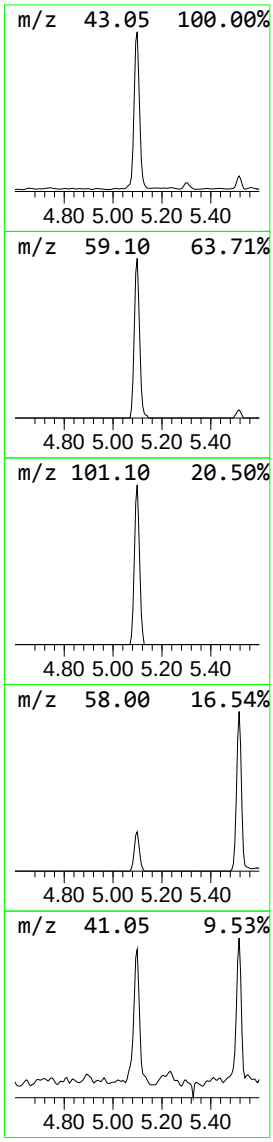
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	2.03 ng	74303	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	25
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Operator : RC/JU
Sample : P4807-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BF-F14

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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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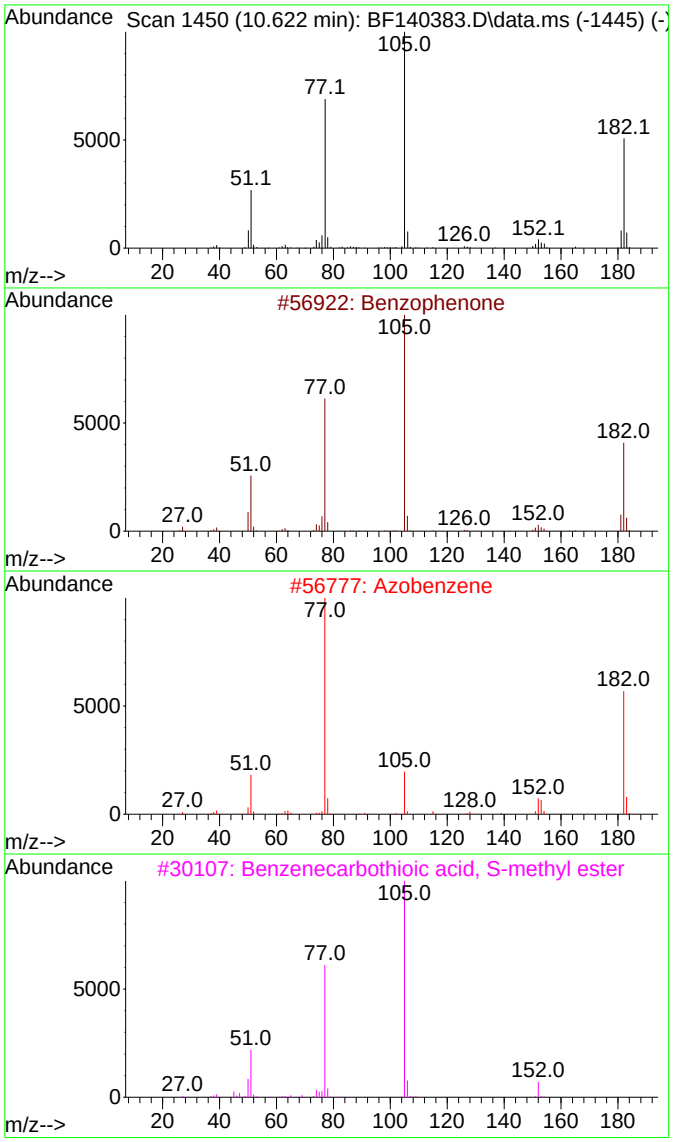
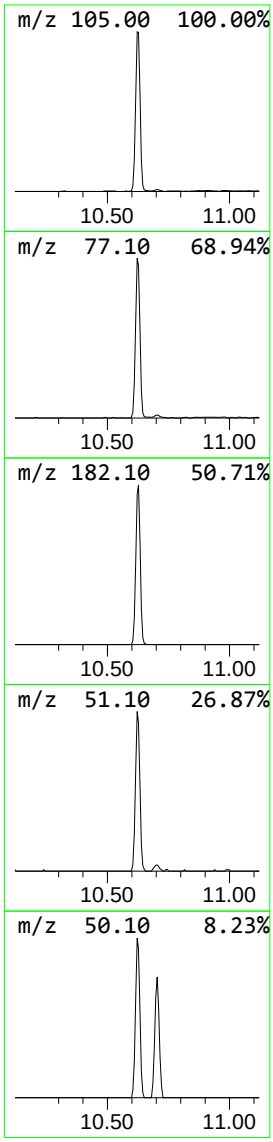
Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.621	6.60 ng	274118	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	72
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47





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Data File : BF140383.D
Acq On : 15 Nov 2024 00:32
Operator : RC/JU
Sample : P4807-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BF-F14

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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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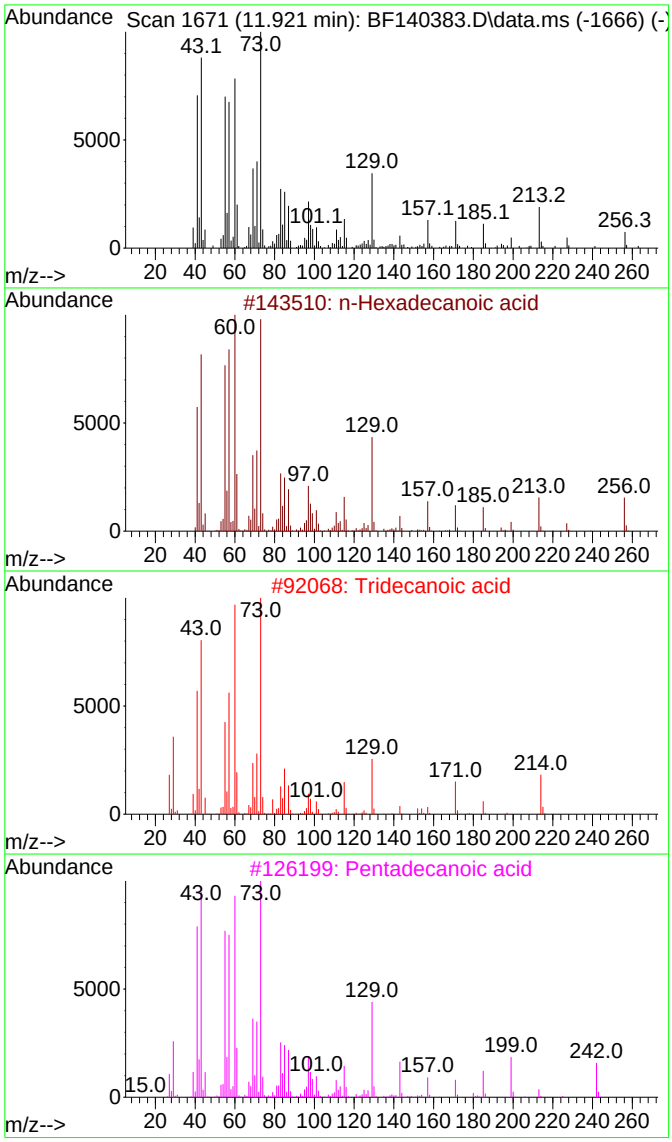
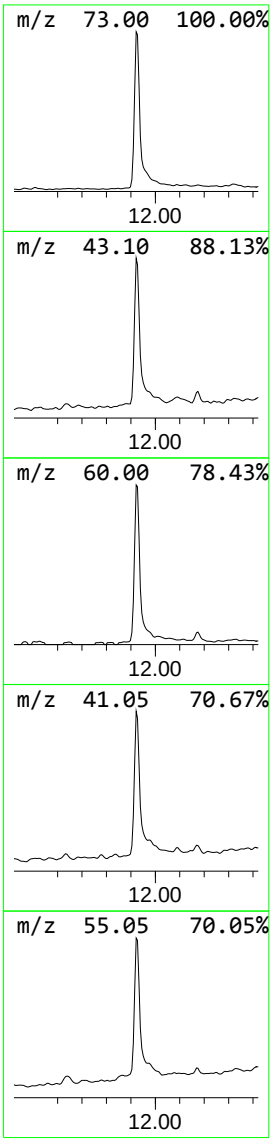
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.921	8.78 ng	327223	Phenanthrene-d10	11.404

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111424\
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Acq On : 15 Nov 2024 00:32
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Sample : P4807-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BF-F14

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
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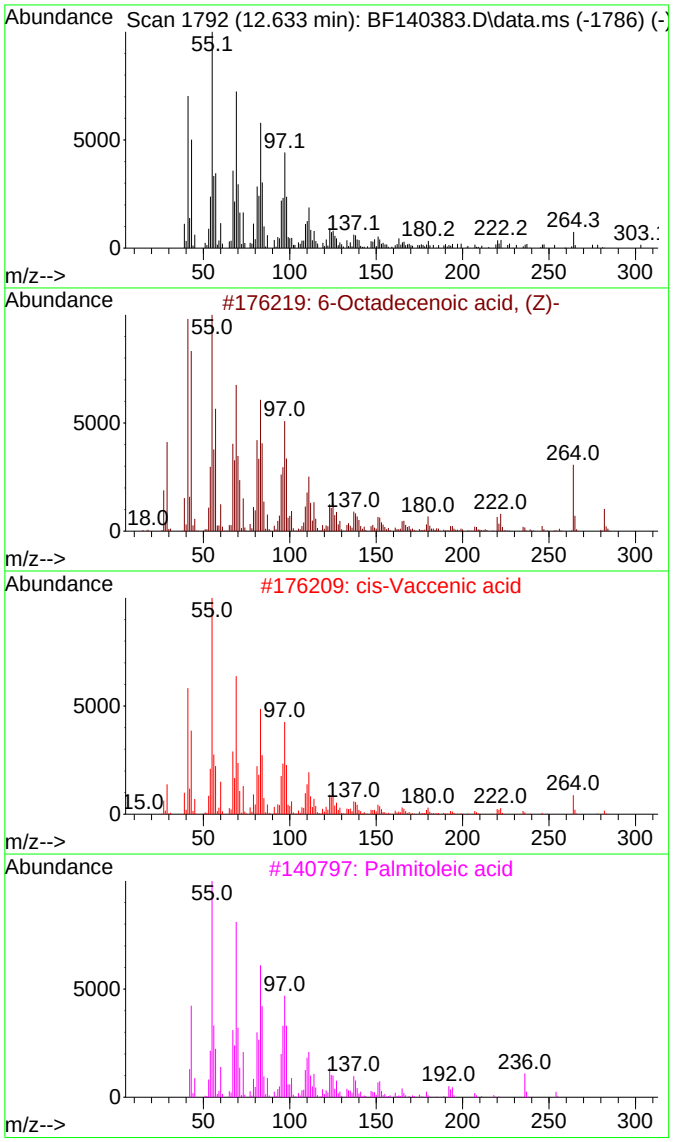
TIC Integration Parameters: LSCINT.P

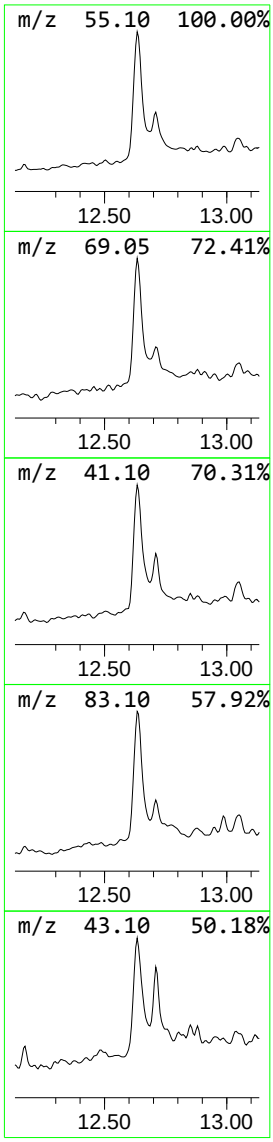
****

Peak Number 5 6-Octadecenoic acid, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	9.41 ng	350856	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	91
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	90
3	Palmitoleic acid	254	C16H30O2	000373-49-9	83
4	Oleic Acid	282	C18H34O2	000112-80-1	83
5	cis-10-Nonadecenoic acid	296	C19H36O2	073033-09-7	83





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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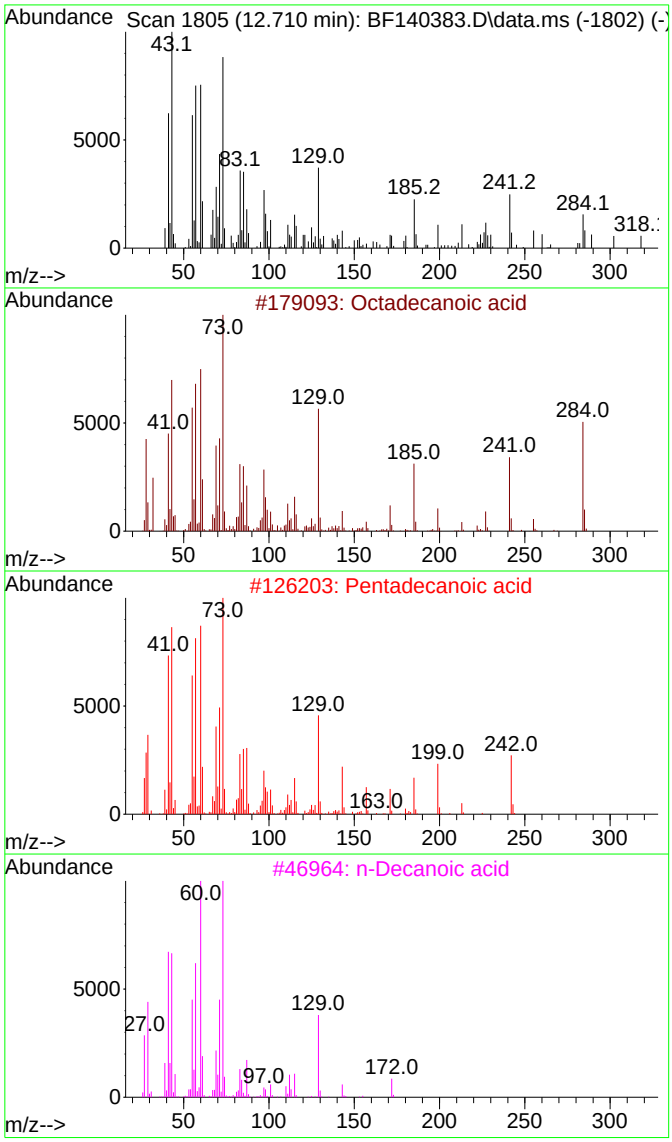
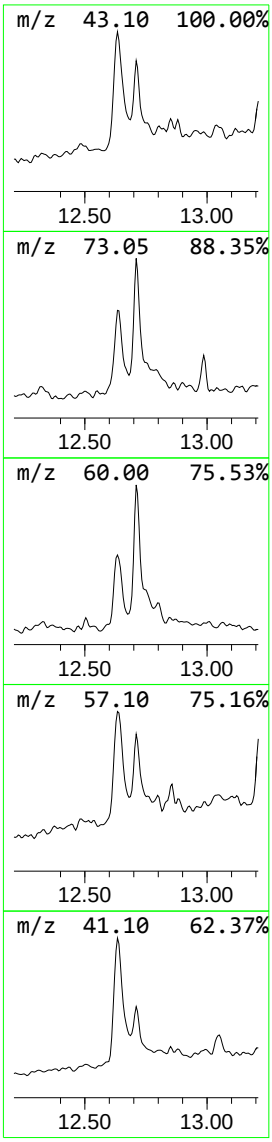
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	2.71 ng	101055	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Dodecanoic acid	200	C12H24O2	000143-07-7	46





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Instrument :
BNA_F
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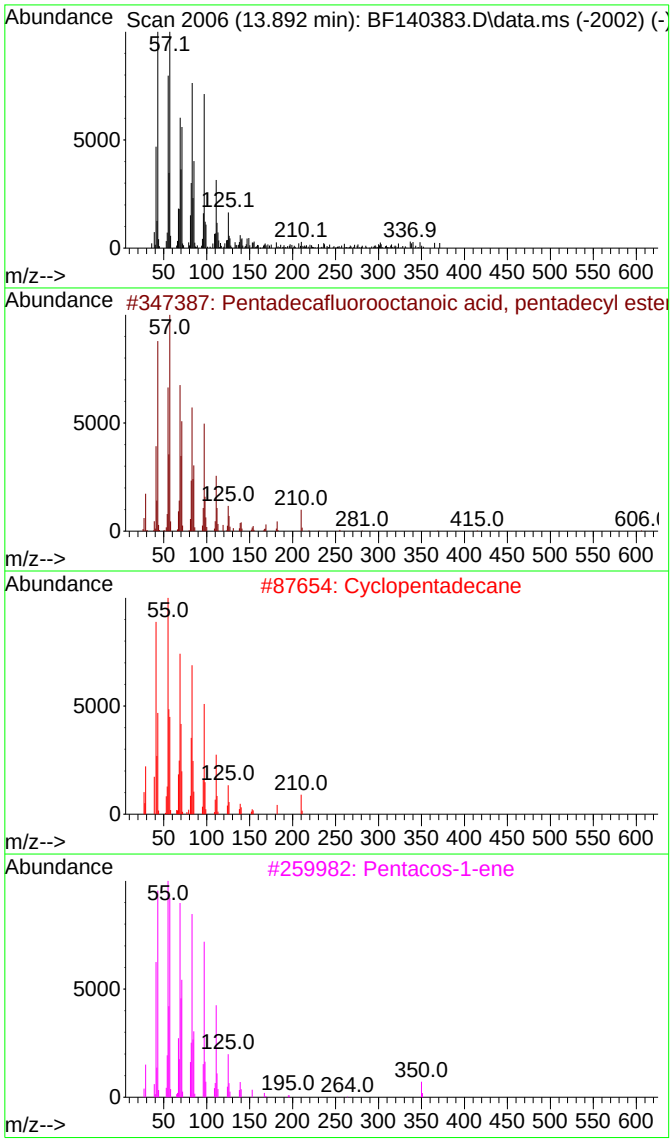
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

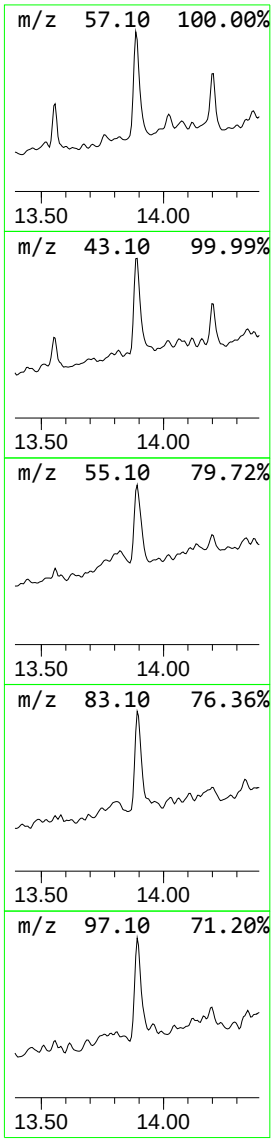
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	5.97 ng	154480	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	94
2	Cyclopentadecane	210	C15H30	000295-48-7	93
3	Pentacos-1-ene	350	C25H50	016980-85-1	93
4	Cyclotetracosane	336	C24H48	000297-03-0	91
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91





Tentatively Identified Compound (LSC) summary

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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...	2.151	37.8	ng	1387370	1	6.875	733498	20.0
2-Pentanone, 4-...	5.098	2.0	ng	74303	1	6.875	733498	20.0
Benzophenone	10.621	6.6	ng	274118	3	9.910	830225	20.0
n-Hexadecanoic ...	11.921	8.8	ng	327223	4	11.404	745710	20.0
6-Octadecenoic ...	12.633	9.4	ng	350856	4	11.404	745710	20.0
Octadecanoic acid	12.710	2.7	ng	101055	4	11.404	745710	20.0
Pentadecafluoro...	13.892	6.0	ng	154480	5	14.045	517605	20.0