LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111424\
Data File : BF140372.D
Acq On : 14 Nov 2024 19:43
Operator : RC/JU
Sample : P4788-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-G3

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: BF140372.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	16	rVB	766131	1206528	43.90%	6.141%
2	2.252	22	27	32	rBV	39223	60326	2.19%	0.307%
3	5.093	504	510	518	rVB	148641	218189	7.94%	1.110%
4	5.504	574	580	601	rVB	1794925	2339695	85.12%	11.908%
5	6.516	745	752	765	rVB	1778221	2477166	90.12%	12.607%
6	6.869	807	812	818	rBV	519548	662875	24.12%	3.374%
7	7.434	902	908	913	rBV	1187864	1552601	56.49%	7.902%
8	7.681	946	950	957	rBV	65582	86058	3.13%	0.438%
9	8.151	1025	1030	1045	rVB	666876	833157	30.31%	4.240%
10	8.363	1060	1066	1076	rBV	24794	35938	1.31%	0.183%
11	9.228	1207	1213	1218	rBV	2138912	2748641	100.00%	13.989%
12	9.904	1323	1328	1334	rBV	643860	821211	29.88%	4.180%
13	10.622	1444	1450	1457	rBV	280512	358557	13.04%	1.825%
14	10.698	1457	1463	1477	rBV	1019732	1318795	47.98%	6.712%
15	10.928	1495	1502	1508	rBV2	16906	31493	1.15%	0.160%
16	11.392	1576	1581	1589	rBV	558614	724486	26.36%	3.687%
17	11.916	1665	1670	1685	rBV2	126543	278569	10.13%	1.418%
18	12.622	1784	1790	1800	rBV	263575	566889	20.62%	2.885%
19	12.980	1846	1851	1856	rBV	1700310	2134972	77.67%	10.866%
20	13.886	2001	2005	2016	rBV	61263	118552	4.31%	0.603%
21	14.045	2027	2032	2038	rVB	452045	591399	21.52%	3.010%
22	15.545	2282	2287	2298	rVB	279371	482424	17.55%	2.455%

Sum of corrected areas: 19648521

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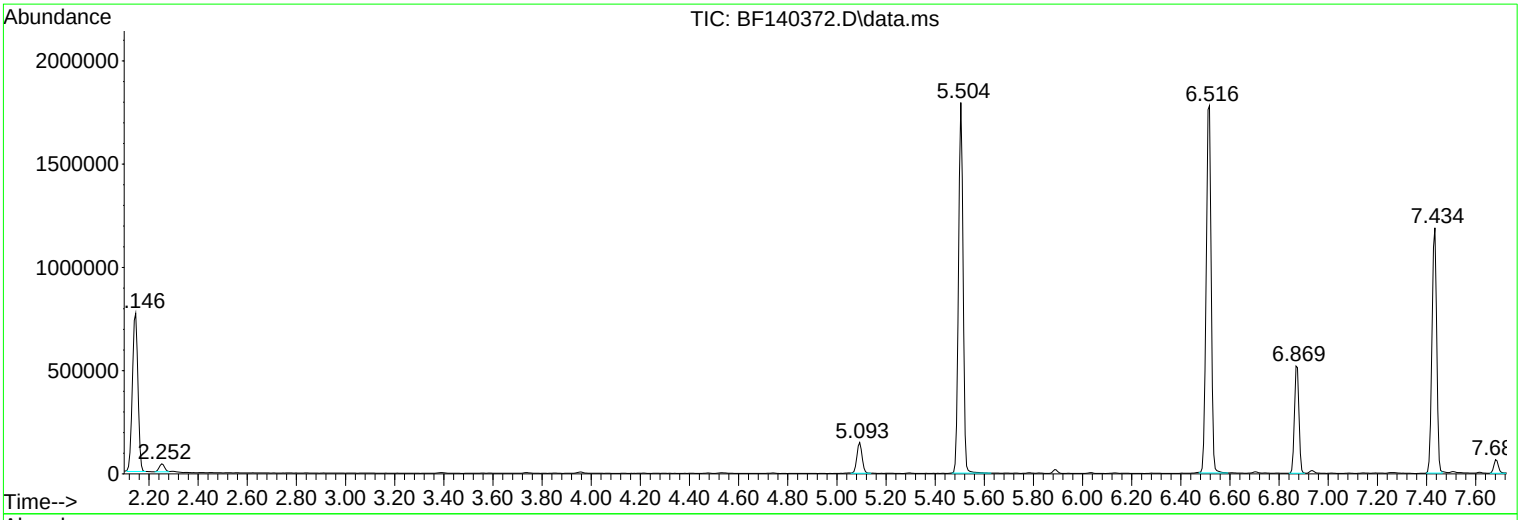
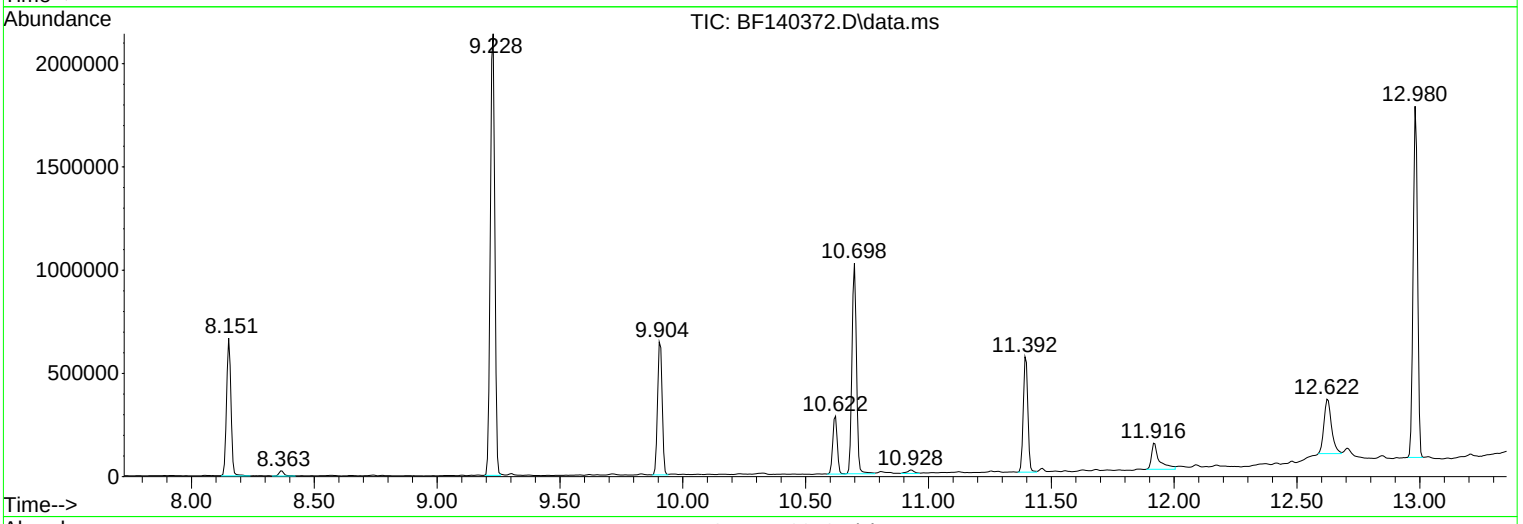
Misc :
ALS Vial : 8 Sample Multiplier: 1

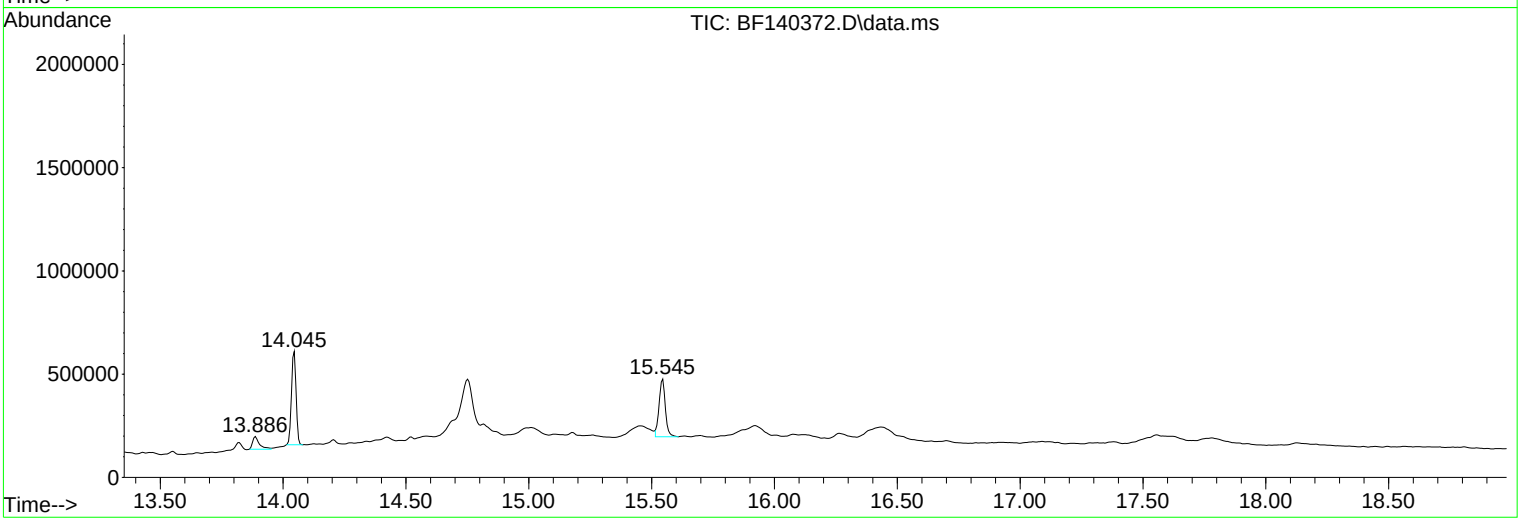
Instrument :
BNA_F
ClientSampleId :
BP-G3

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

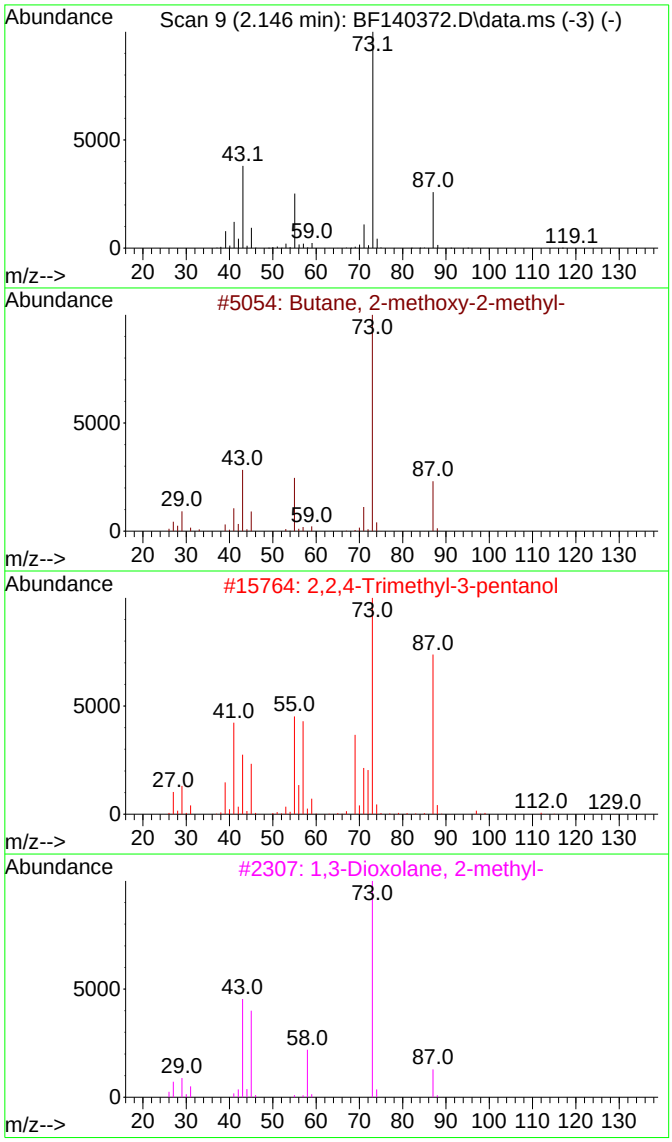
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

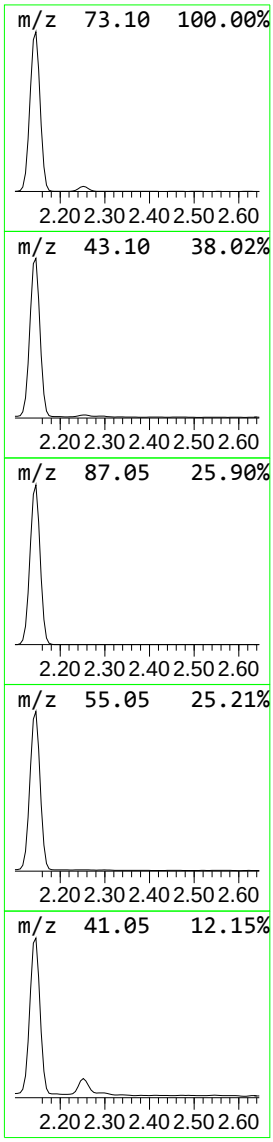
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	36.40 ng	1206530	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	78
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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Instrument :
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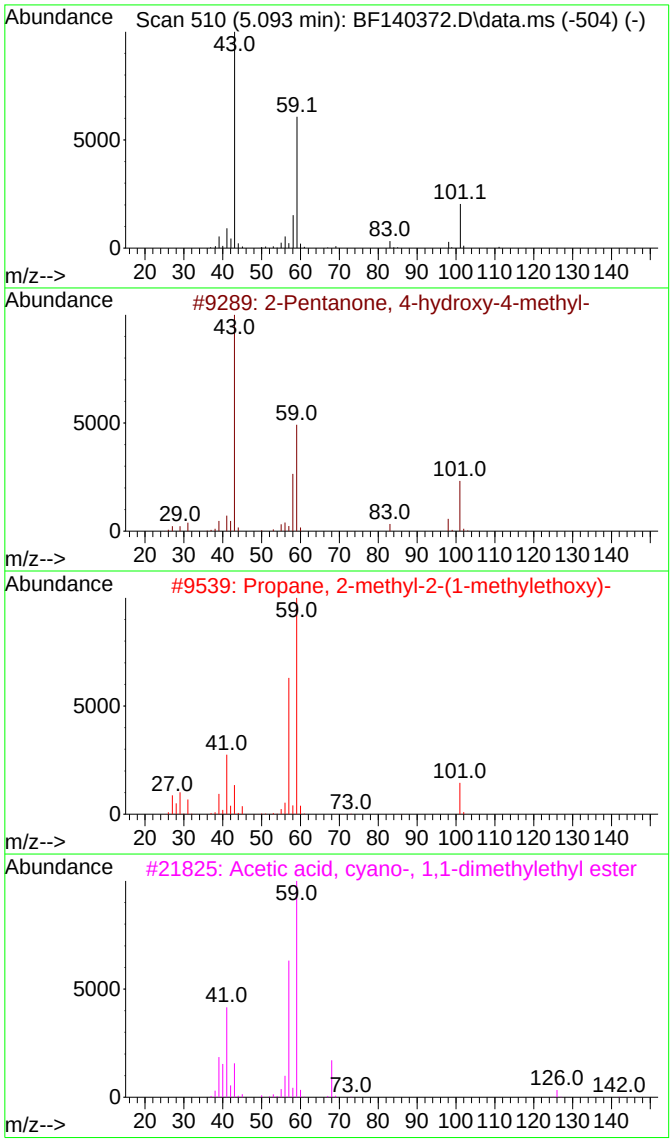
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

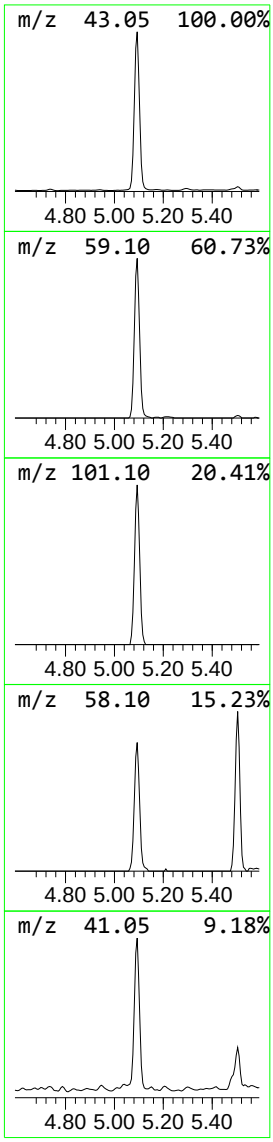
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	6.58 ng	218189	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	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111424\
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Acq On : 14 Nov 2024 19:43
Operator : RC/JU
Sample : P4788-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-G3

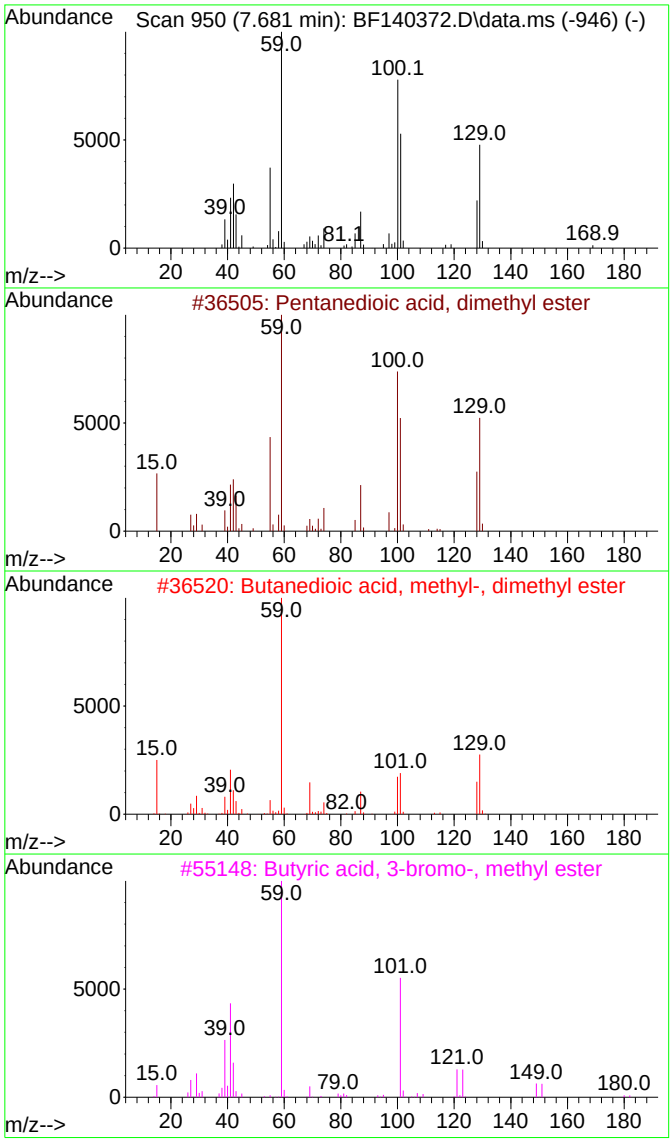
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

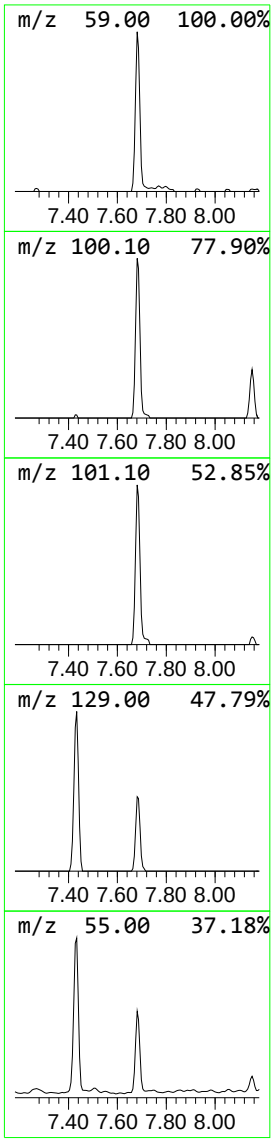
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentanedioic acid, dimethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.681	2.07 ng	86058	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	91
2	Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	50
3	Butyric acid, 3-bromo-, methyl e...	180	C5H9BrO2	021249-59-2	27
4	1,4-Di-O-acetyl-2,5-di-O-methyl-...	262	C12H22O6	1000101-82-1	25
5	Butanoic acid, 4-(2-methoxy-1-me...	204	C9H16O5	054966-46-0	23





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Sample : P4788-01
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
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TIC Library : C:\Database\NIST20.L
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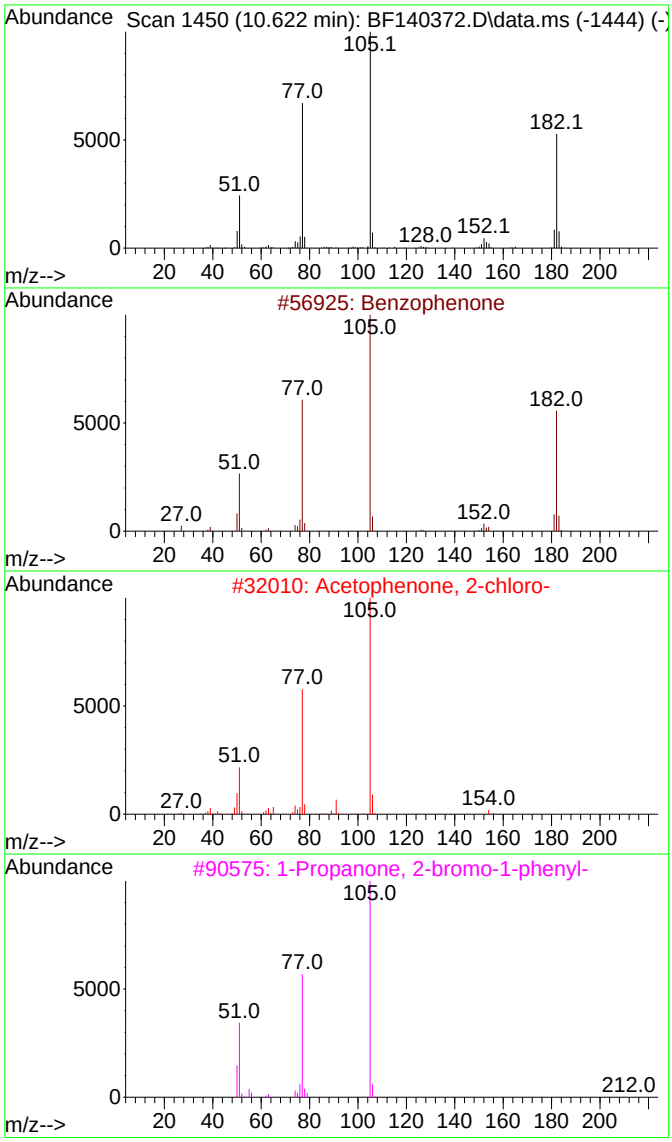
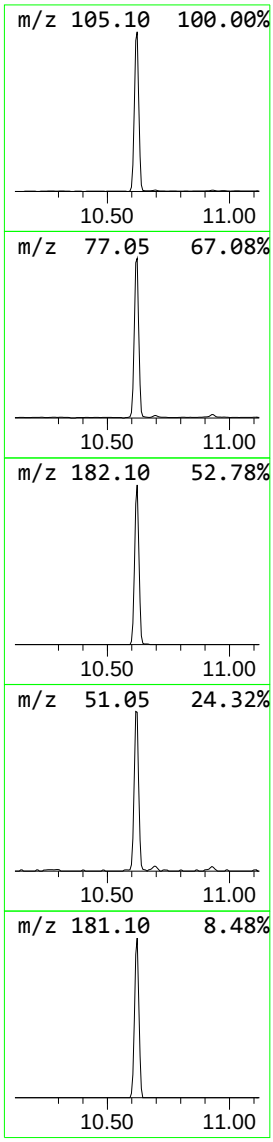
****

Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	8.73 ng	358557	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5	Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47





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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

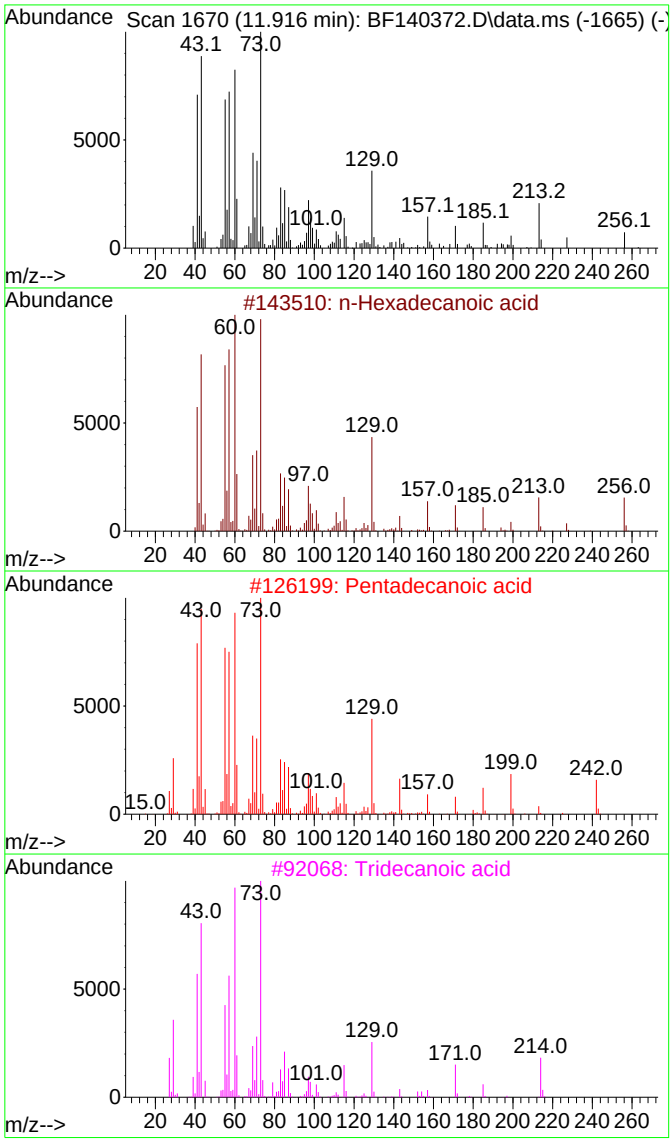
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

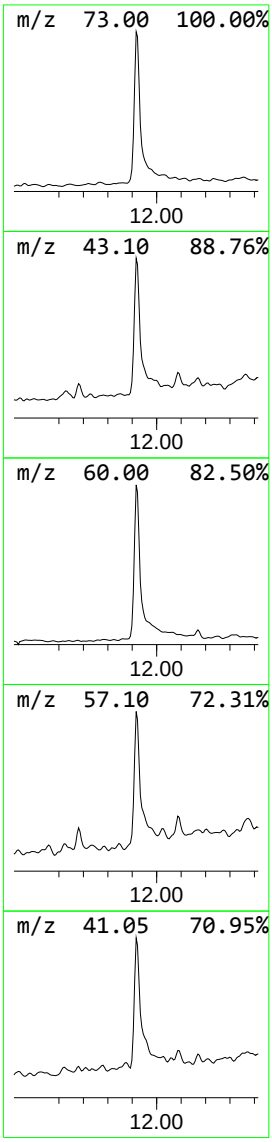
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	7.69 ng	278569	Phenanthrene-d10	11.392

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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Nonanoic acid	158	C9H18O2	000112-05-0	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

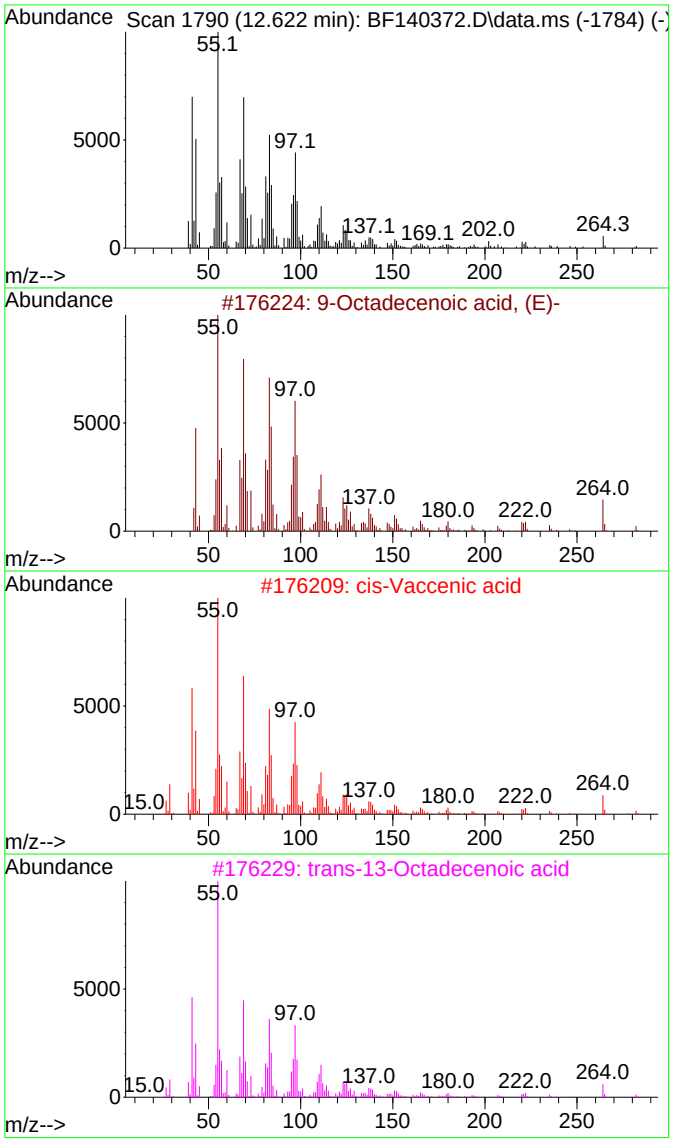
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

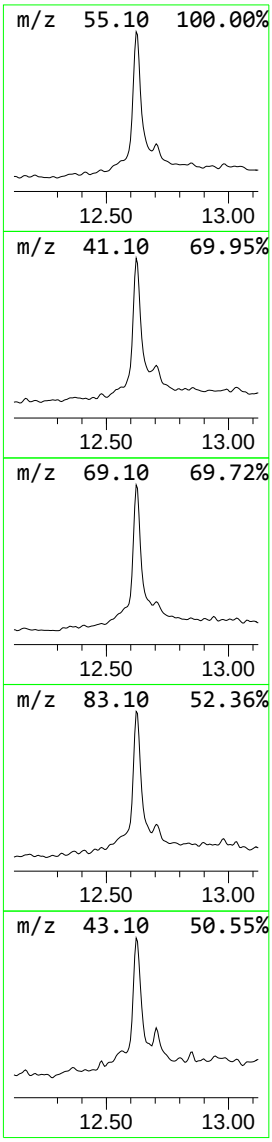
****

Peak Number 6 9-Octadecenoic acid, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.622	15.65 ng	566889	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	99
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	98
3	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	98
4	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	97
5	Oleic Acid	282	C18H34O2	000112-80-1	96





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

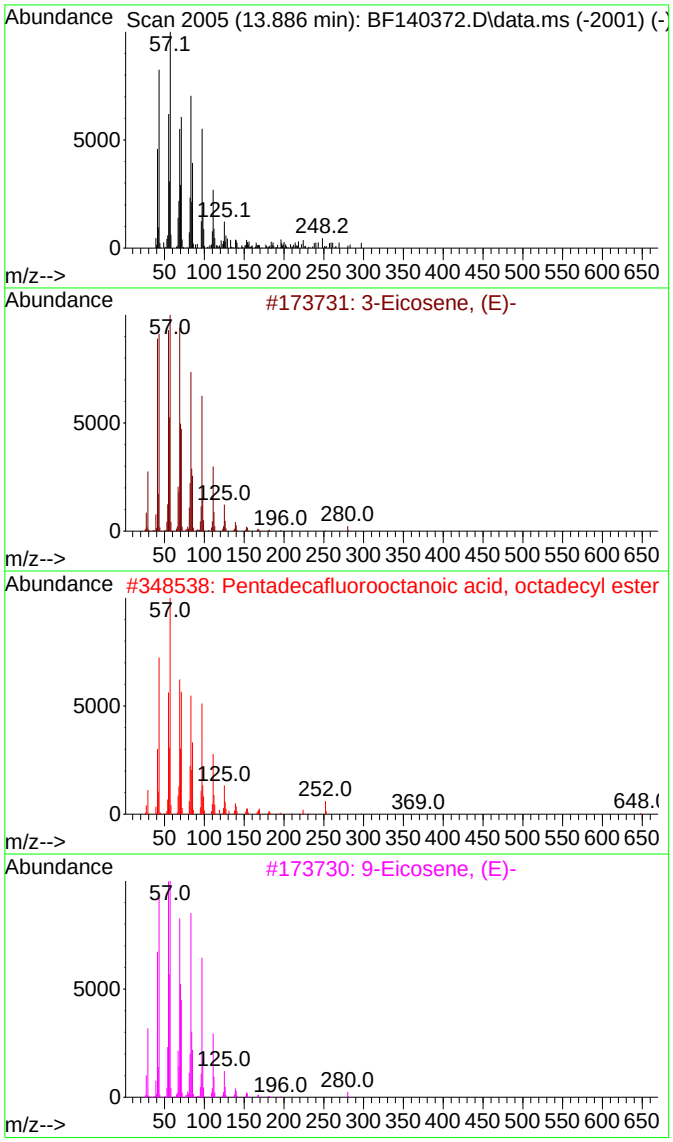
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

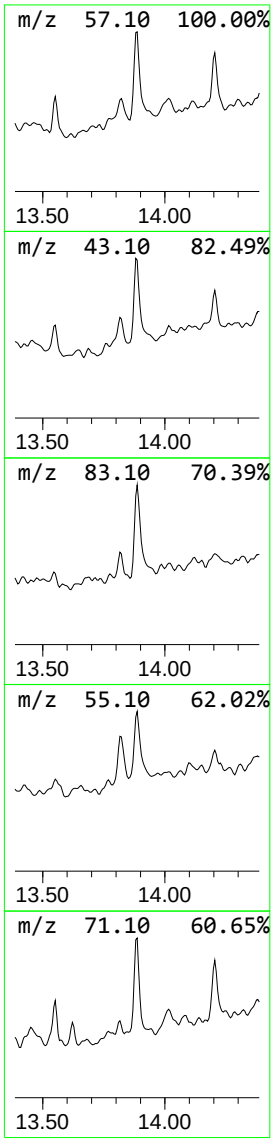
****

Peak Number 7 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	4.01 ng	118552	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	92
5	Cyclotetradecane	196	C14H28	000295-17-0	91





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.146	36.4	ng	1206530	1	6.875	662875	20.0
2-Pentanone, 4-...	5.093	6.6	ng	218189	1	6.875	662875	20.0
Pentanedioic ac...	7.681	2.1	ng	86058	2	8.151	833157	20.0
Benzophenone	10.622	8.7	ng	358557	3	9.904	821211	20.0
n-Hexadecanoic ...	11.916	7.7	ng	278569	4	11.392	724486	20.0
9-Octadecenoic ...	12.622	15.7	ng	566889	4	11.392	724486	20.0
3-Eicosene, (E)-	13.886	4.0	ng	118552	5	14.045	591399	20.0