LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011425\
Data File : BF141154.D
Acq On : 14 Jan 2025 19:04
Operator : RC/JU
Sample : Q1074-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HACKENSACK-DGA

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-BF011025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141154.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	5	12	rVB	1003738	1174663	27.19%	3.678%
2	2.222	17	22	34	rVB	73503	119039	2.75%	0.373%
3	5.040	491	501	510	rVB	143421	229725	5.32%	0.719%
4	5.434	561	568	573	rBV	2605508	3561021	82.41%	11.151%
5	6.440	733	739	745	rVV	2492476	3588519	83.05%	11.237%
6	6.816	798	803	809	rBV	707047	884587	20.47%	2.770%
7	7.375	892	898	904	rBV	1672646	2401069	55.57%	7.518%
8	7.634	937	942	947	rBV	74766	94641	2.19%	0.296%
9	8.098	1015	1021	1030	rBV	915543	1210815	28.02%	3.791%
10	8.316	1052	1058	1066	rVB	34492	47452	1.10%	0.149%
11	9.175	1197	1204	1210	rBV	3164448	4320995	100.00%	13.530%
12	9.851	1311	1319	1325	rBV	1011517	1356325	31.39%	4.247%
13	10.569	1436	1441	1447	rVB	263543	331420	7.67%	1.038%
14	10.639	1447	1453	1467	rBV	2192708	3037173	70.29%	9.510%
15	11.339	1567	1572	1580	rBV	1023875	1401532	32.44%	4.389%
16	11.874	1654	1663	1673	rBV2	763064	1187256	27.48%	3.718%
17	11.951	1673	1676	1685	rVB	48889	105108	2.43%	0.329%
18	12.133	1703	1707	1715	rVB4	27577	54354	1.26%	0.170%
19	12.551	1774	1778	1785	rBV	171546	239826	5.55%	0.751%
20	12.657	1791	1796	1810	rBV2	189139	320216	7.41%	1.003%
21	12.780	1812	1817	1823	rVV	167102	227459	5.26%	0.712%
22	12.927	1837	1842	1849	rVB	2772433	3680359	85.17%	11.524%
23	13.839	1992	1997	2011	rVB2	159402	296698	6.87%	0.929%
24	13.980	2015	2021	2036	rVV2	699167	1125017	26.04%	3.523%
25	15.374	2255	2258	2263	rVB	62886	85153	1.97%	0.267%
26	15.439	2264	2269	2283	rVB	510498	855149	19.79%	2.678%

Sum of corrected areas: 31935571

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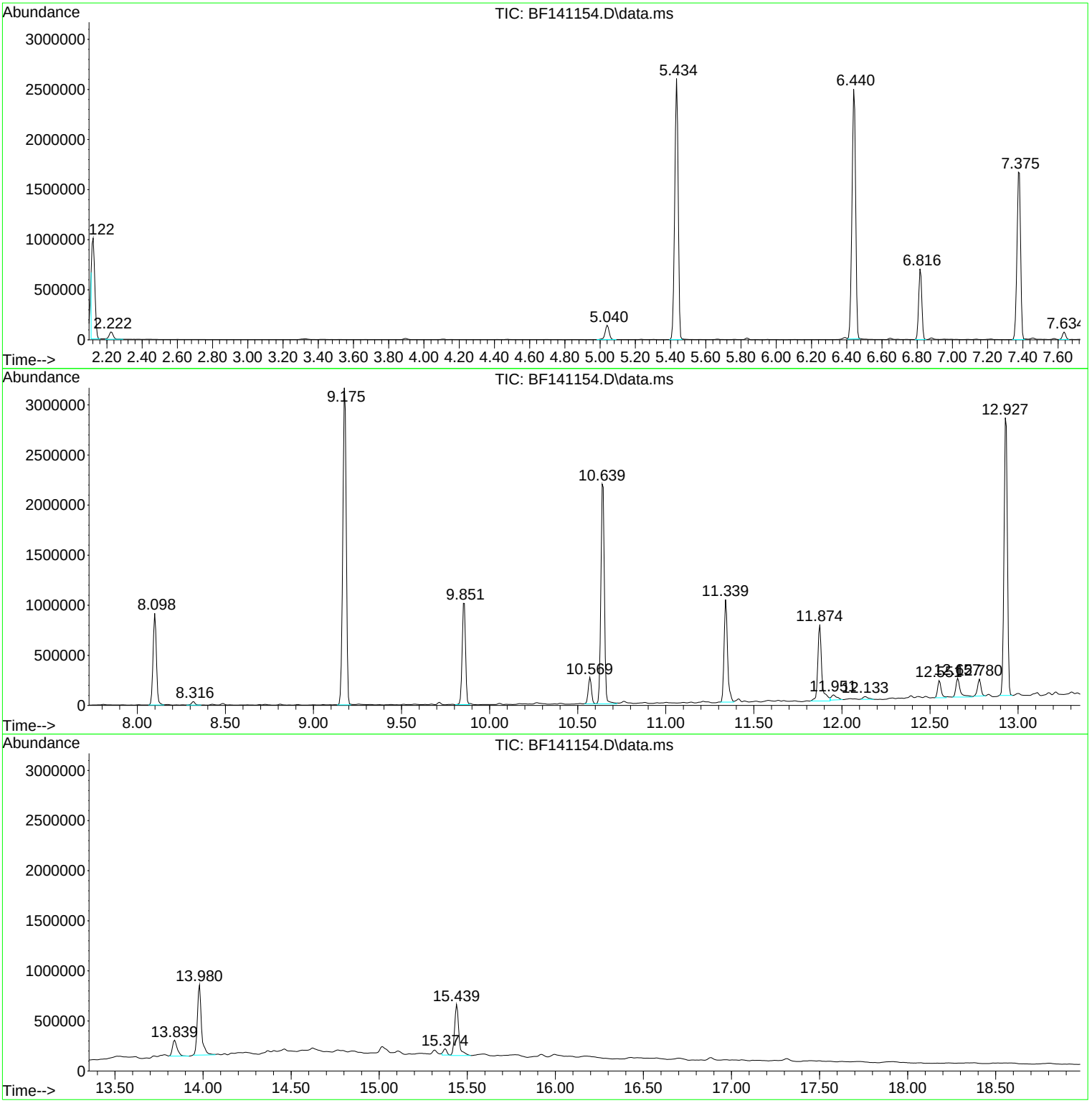
ClientSampleId :
HACKENSACK-DGA

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011425\
Data File : BF141154.D
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Operator : RC/JU
Sample : Q1074-01
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ClientSampleId :
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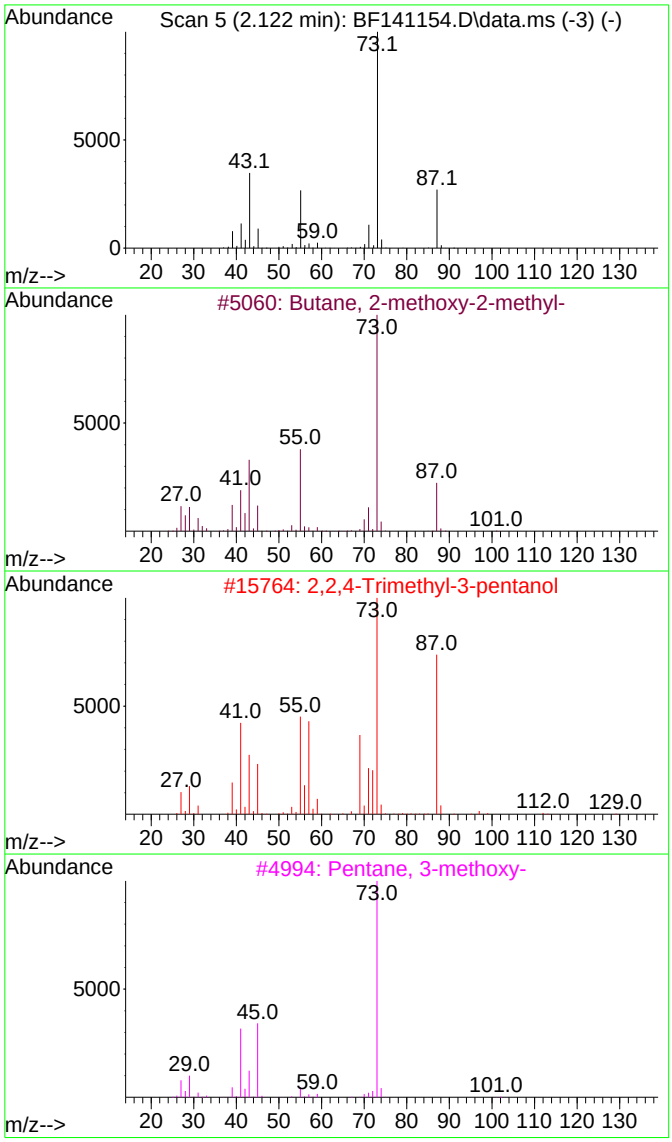
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

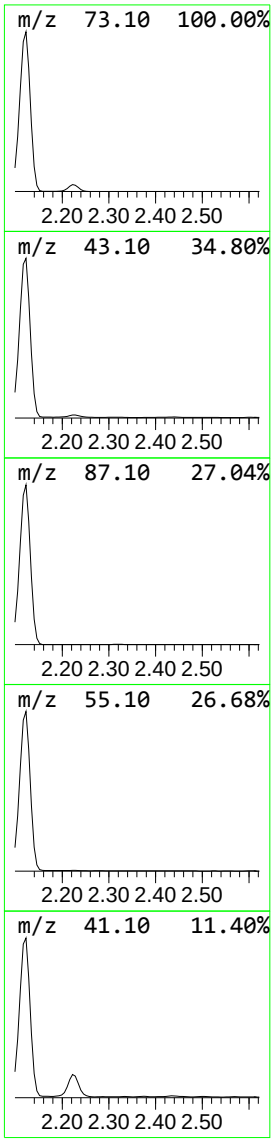
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	26.56 ng	1174660	1,4-Dichlorobenzene-d4	6.816

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	36
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Data File : BF141154.D
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Operator : RC/JU
Sample : Q1074-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HACKENSACK-DGA

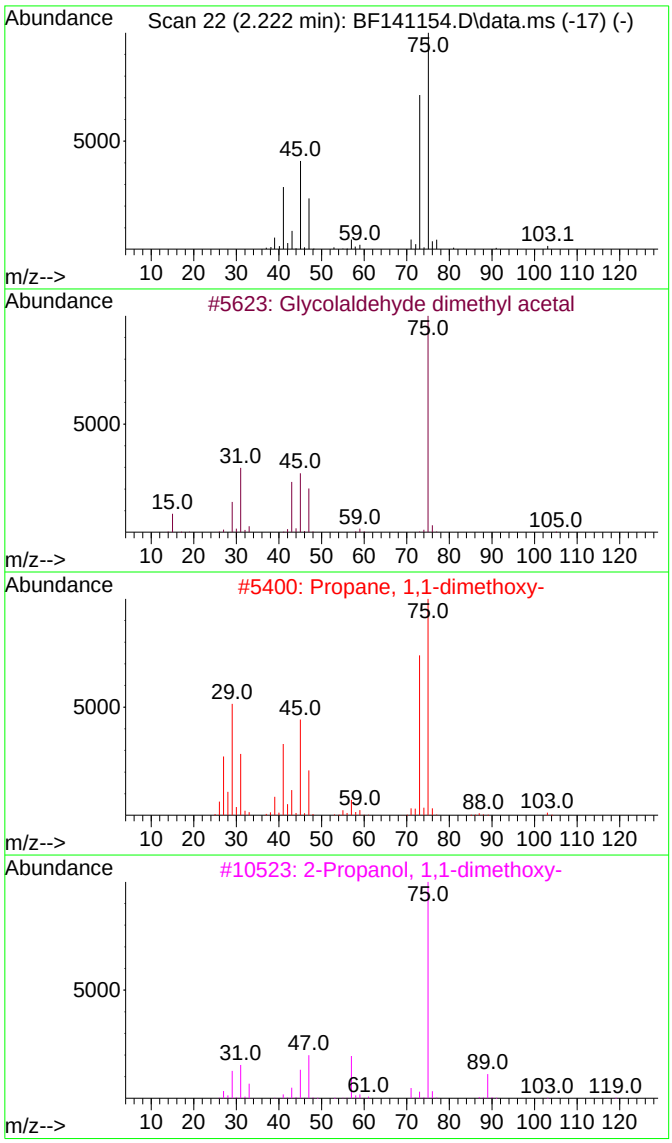
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

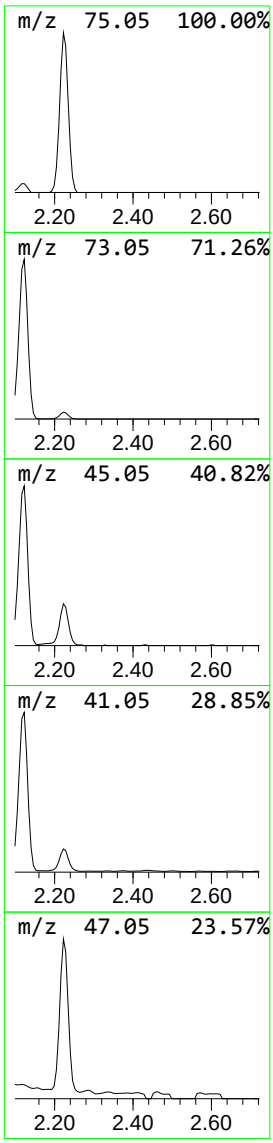
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Glycolaldehyde dimethyl acetal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	2.69 ng	119039	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	72
2	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	43
3	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	36
4	Methane, trimethoxy-	106	C4H10O3	000149-73-5	28
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011425\
Data File : BF141154.D
Acq On : 14 Jan 2025 19:04
Operator : RC/JU
Sample : Q1074-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HACKENSACK-DGA

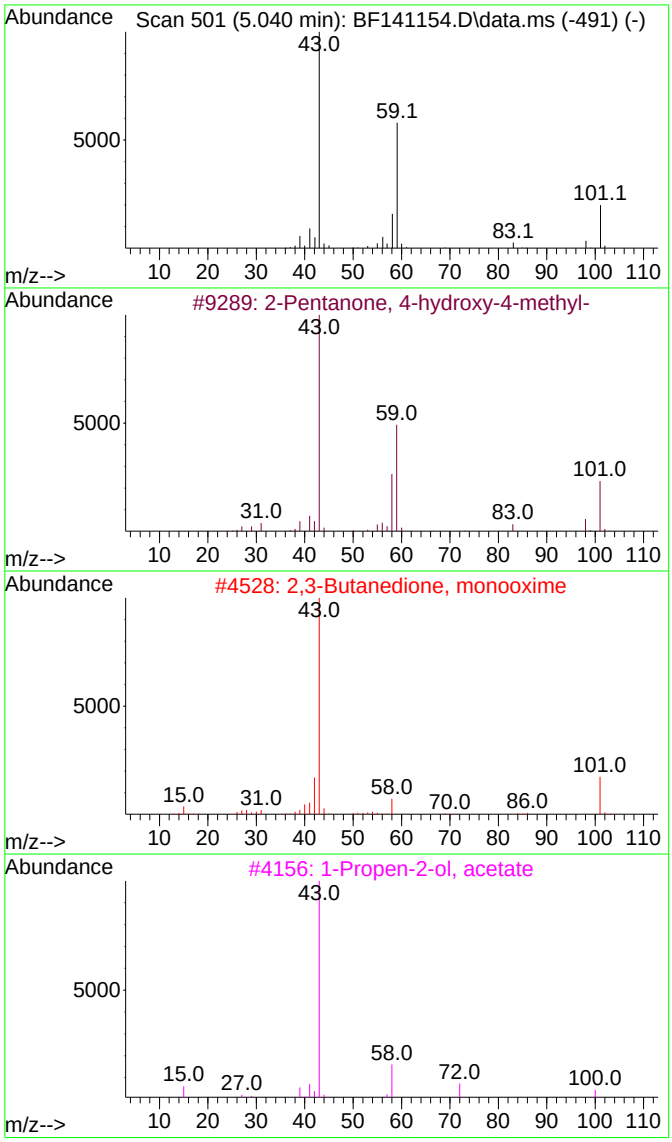
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

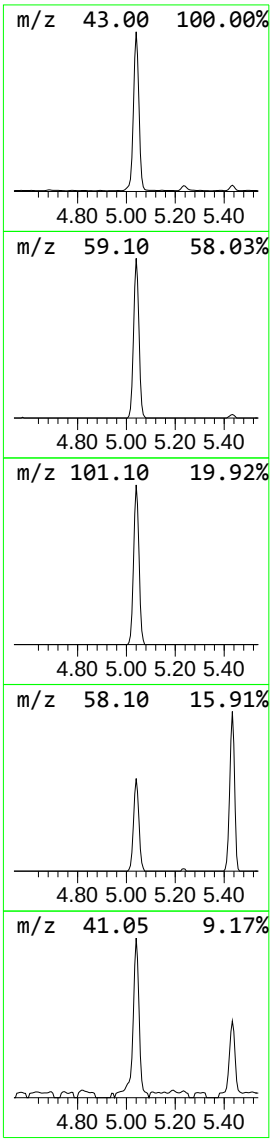
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	5.19 ng	229725	1,4-Dichlorobenzene-d4	6.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Acetone	58	C3H6O	000067-64-1	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Sample : Q1074-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HACKENSACK-DGA

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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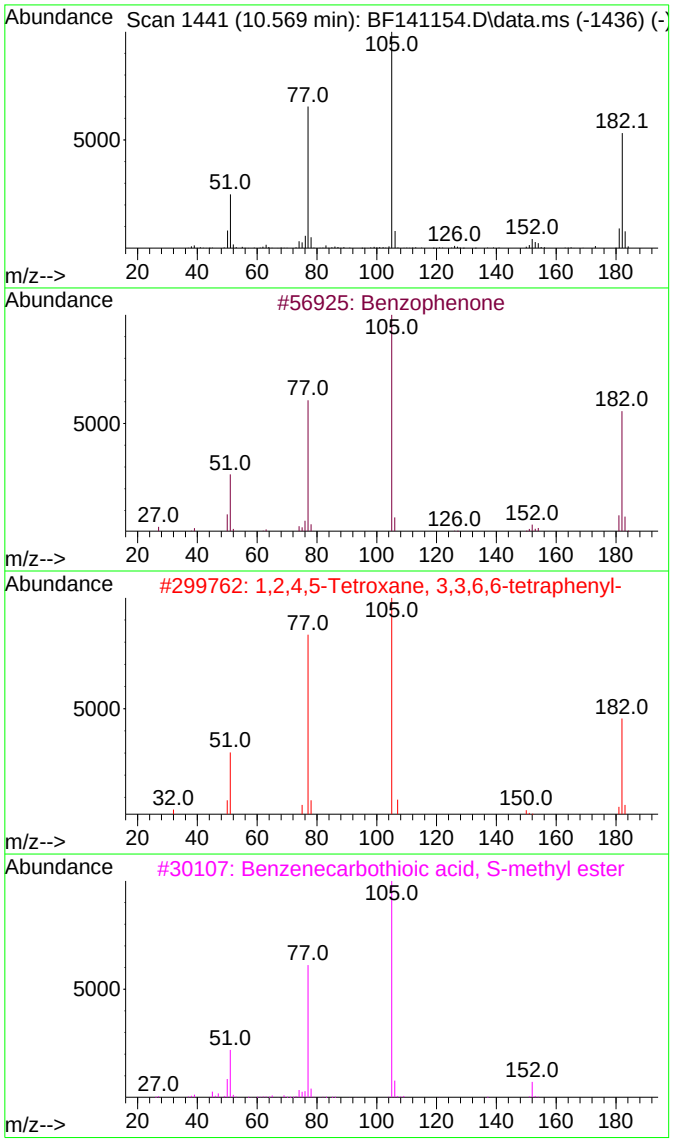
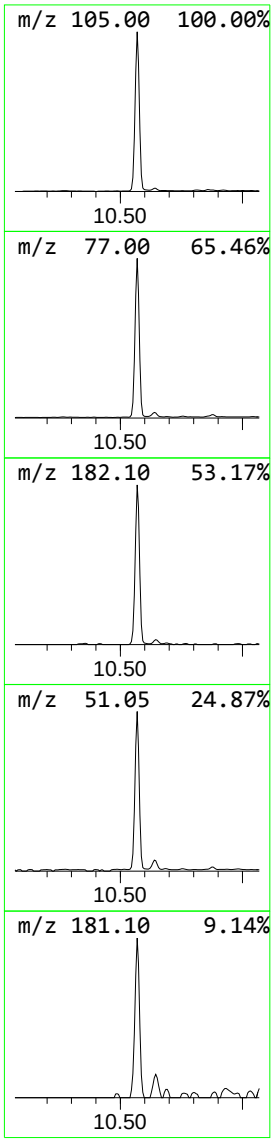
****

Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.569	4.89 ng	331420	Acenaphthene-d10	9.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
4	.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	47
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47





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Sample : Q1074-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HACKENSACK-DGA

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
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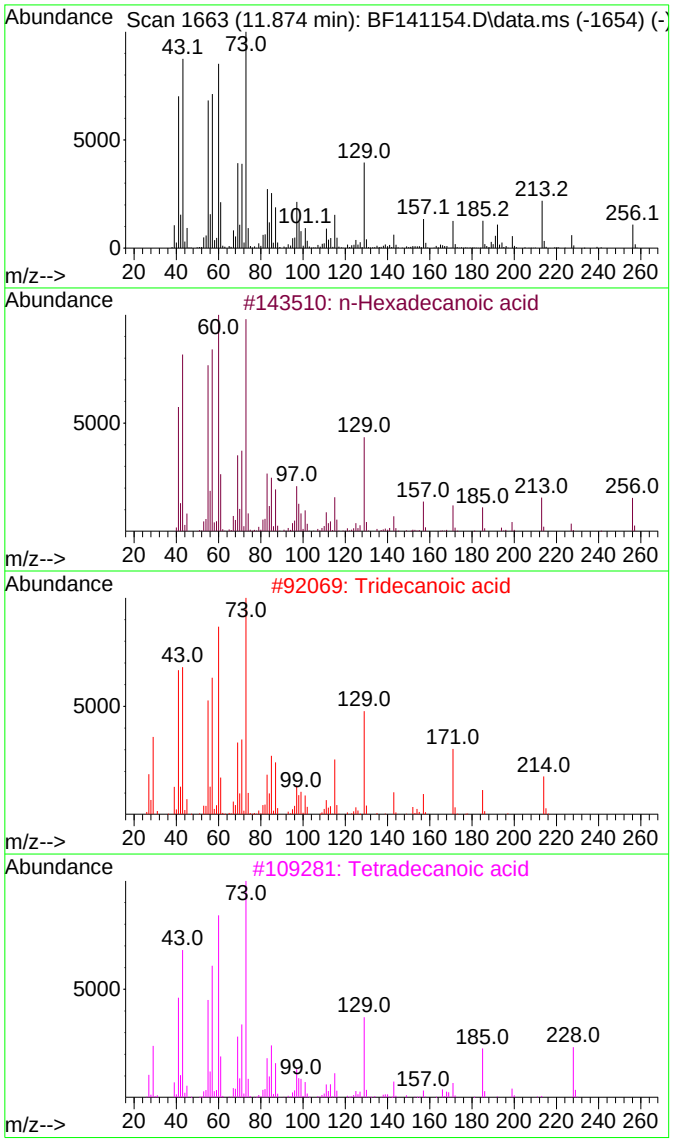
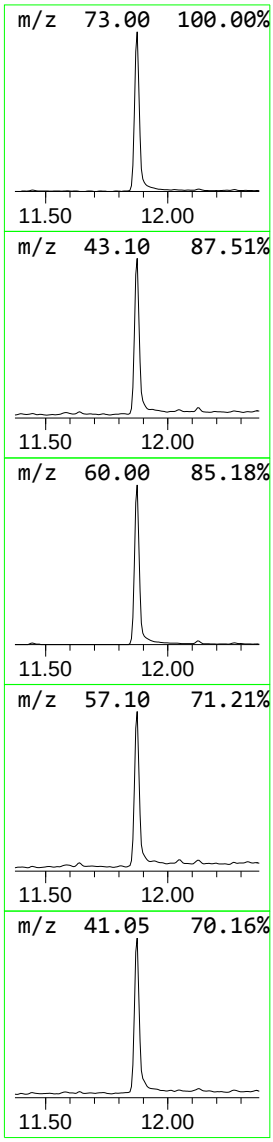
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	16.94 ng	1187260	Phenanthrene-d10	11.339

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	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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BNA_F
ClientSampleId :
HACKENSACK-DGA

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

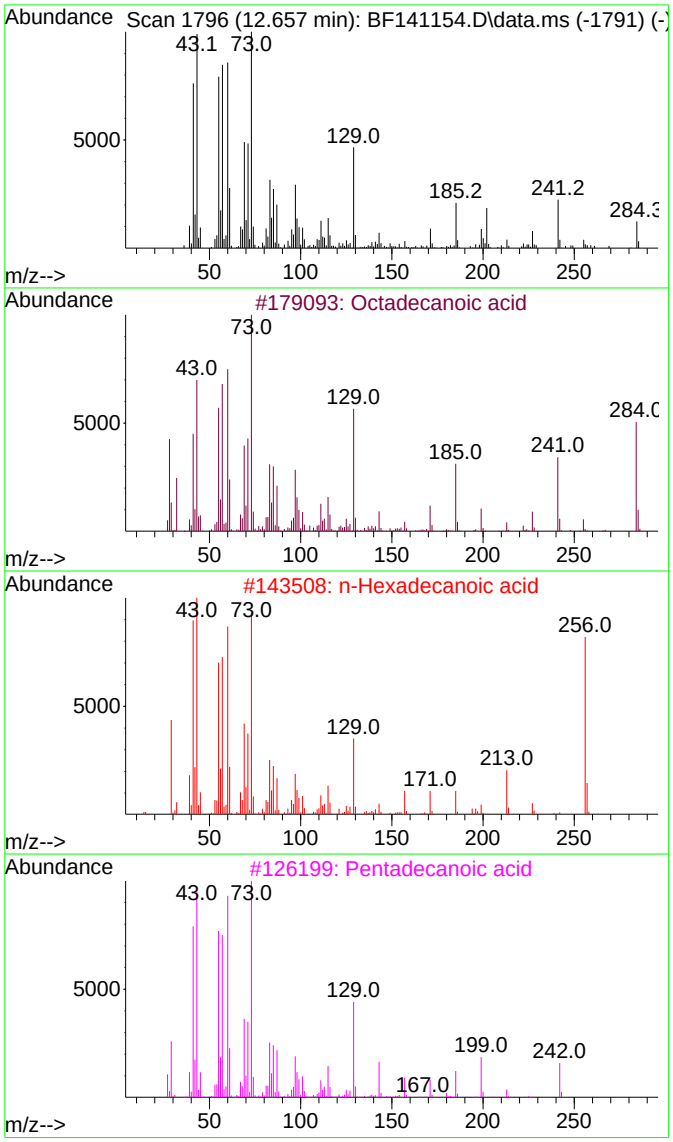
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

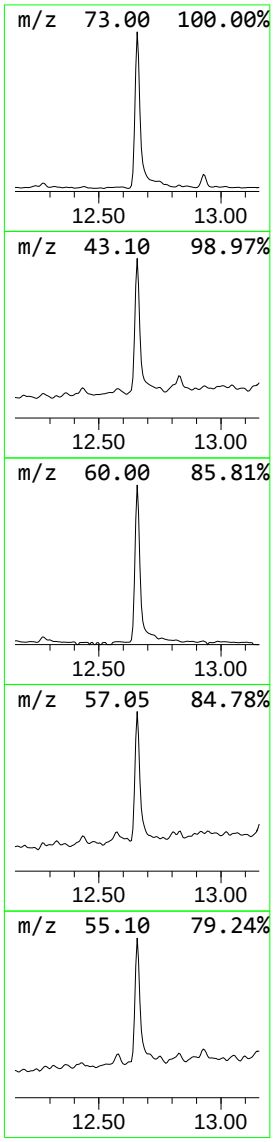
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.657	4.57 ng	320216	Phenanthrene-d10	11.339

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HACKENSACK-DGA

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

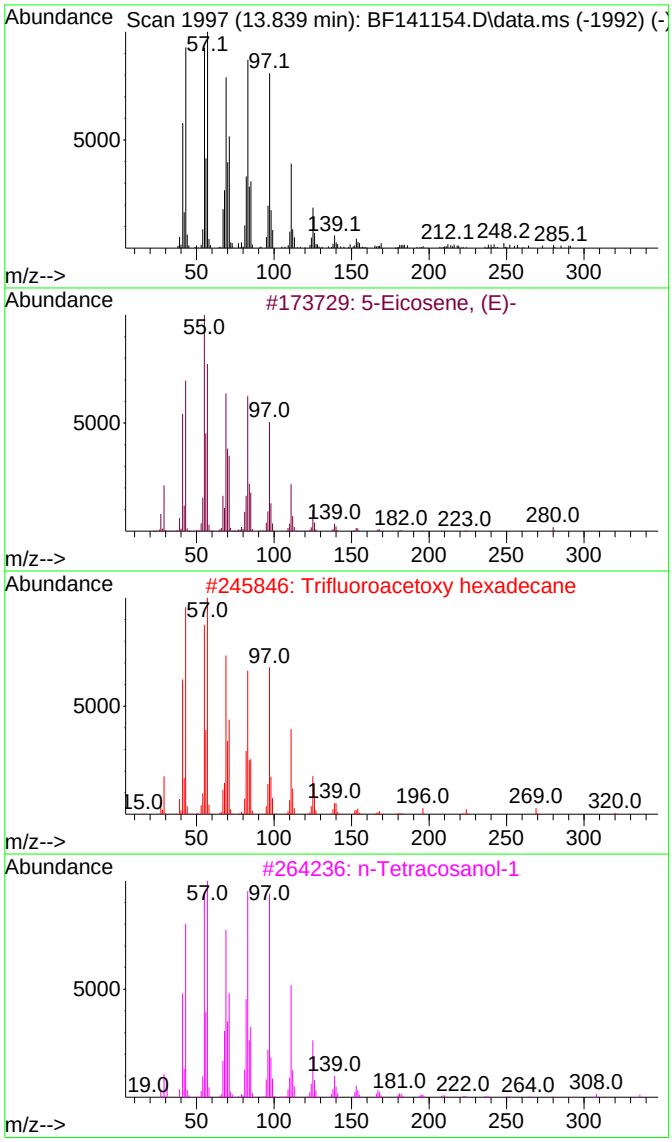
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

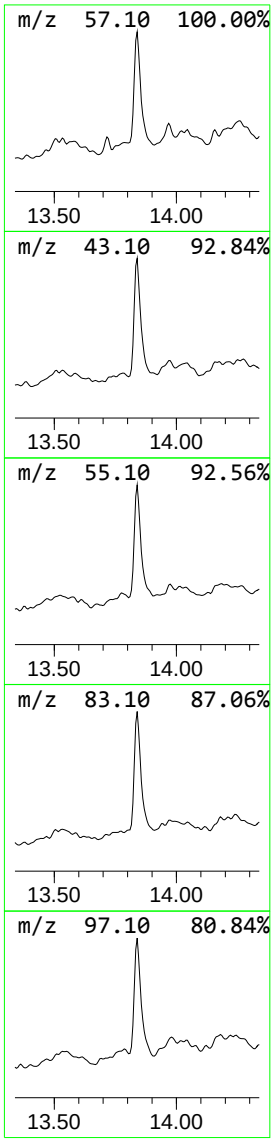
****

Peak Number 7 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	5.27 ng	296698	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	1-Tetracosene	336	C24H48	010192-32-2	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...	2.122	26.6	ng	1174660	1	6.816	884587	20.0
Glycolaldehyde ...	2.222	2.7	ng	119039	1	6.816	884587	20.0
2-Pentanone, 4-...	5.040	5.2	ng	229725	1	6.816	884587	20.0
Benzophenone	10.569	4.9	ng	331420	3	9.857	1356330	20.0
n-Hexadecanoic ...	11.874	16.9	ng	1187260	4	11.339	1401530	20.0
Octadecanoic acid	12.657	4.6	ng	320216	4	11.339	1401530	20.0
5-Eicosene, (E)-	13.839	5.3	ng	296698	5	13.980	1125020	20.0