LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072924\
Data File : BF138671.D
Acq On : 29 Jul 2024 16:11
Operator : RC/JU
Sample : P3393-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-852-GI-SO-9.5-10-072624

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-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138671.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	3	12	24	rVB	1578777	2477538	77.53%	11.029%
2	2.522	60	73	82	rVB	186602	335779	10.51%	1.495%
3	3.393	215	221	239	rBV	48175	122463	3.83%	0.545%
4	5.081	503	508	518	rVB	138238	227059	7.11%	1.011%
5	5.481	570	576	581	rBV	2189548	2917241	91.29%	12.987%
6	6.486	741	747	767	rBV	2163753	3083795	96.50%	13.728%
7	6.845	803	808	814	rVB	496038	632572	19.80%	2.816%
8	7.410	898	904	910	rBV	1348399	1926354	60.28%	8.576%
9	7.663	942	947	953	rBV	60476	74078	2.32%	0.330%
10	8.128	1021	1026	1031	rBV	653141	813572	25.46%	3.622%
11	8.445	1075	1080	1095	rBV	87685	133184	4.17%	0.593%
12	9.210	1203	1210	1215	rBV	2521025	3195532	100.00%	14.226%
13	9.886	1320	1325	1331	rVB	654566	828610	25.93%	3.689%
14	9.980	1335	1341	1349	rBV	98983	155653	4.87%	0.693%
15	10.680	1454	1460	1471	rBV	1084397	1401778	43.87%	6.240%
16	11.374	1573	1578	1586	rBV	522172	662448	20.73%	2.949%
17	11.904	1662	1668	1687	rBV2	74243	163364	5.11%	0.727%
18	12.686	1797	1801	1806	rBV4	21520	42428	1.33%	0.189%
19	12.963	1842	1848	1853	rBV	1640422	2099620	65.70%	9.347%
20	13.868	1997	2002	2014	rBV	105983	251325	7.86%	1.119%
21	14.015	2023	2027	2034	rVB	396341	521379	16.32%	2.321%
22	15.486	2273	2277	2287	rVB	249884	397623	12.44%	1.770%

Sum of corrected areas: 22463395

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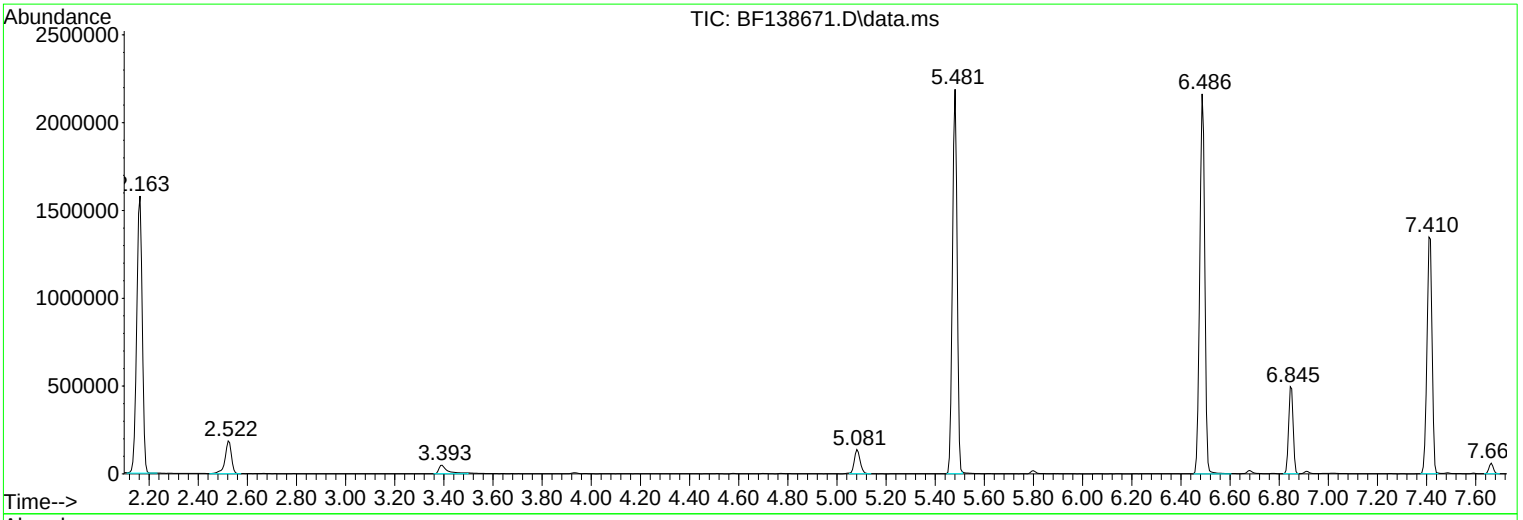
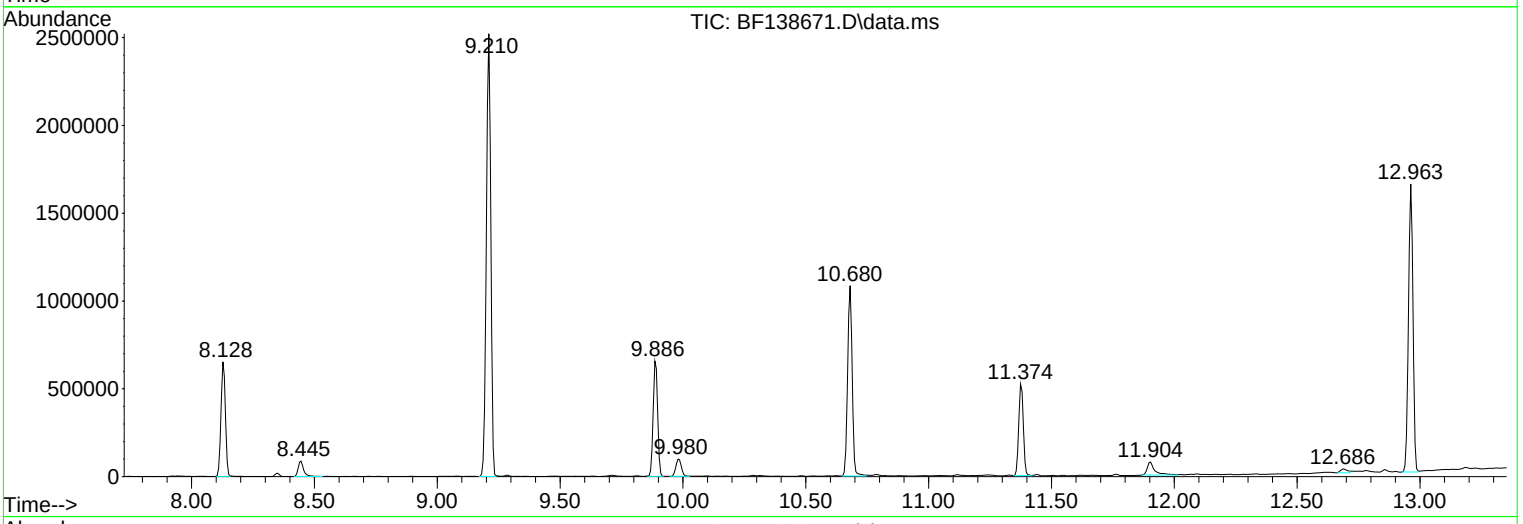
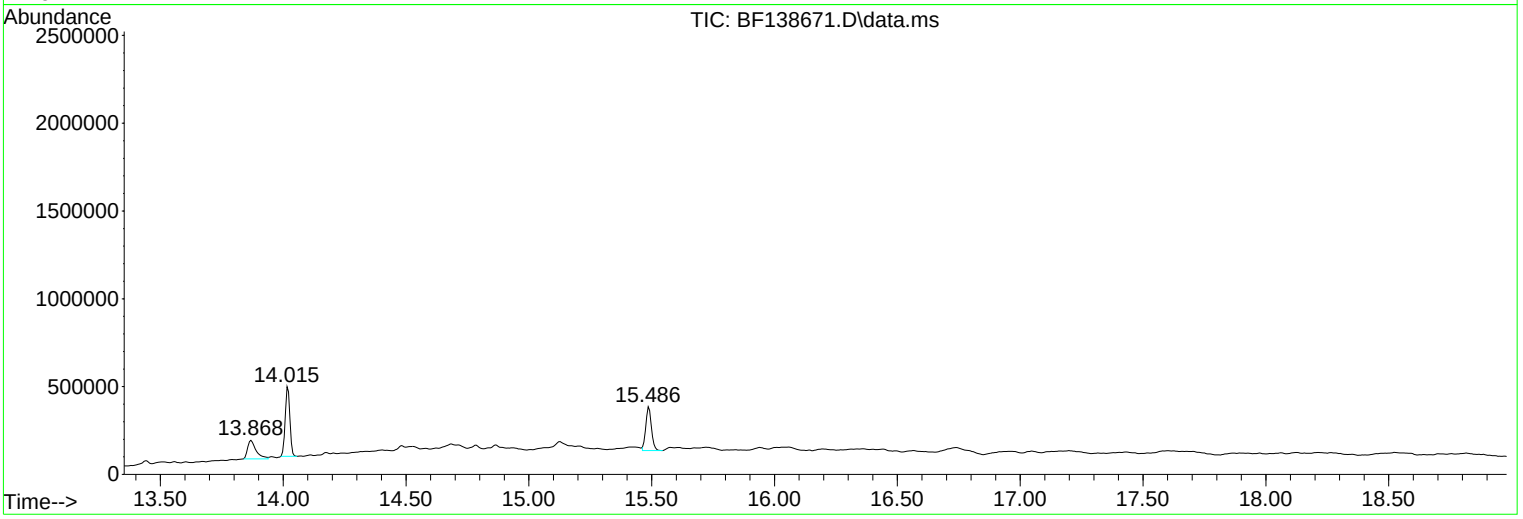
Instrument :
BNA_F
ClientSampleId :
S-852-GI-SO-9.5-10-072624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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Data File : BF138671.D
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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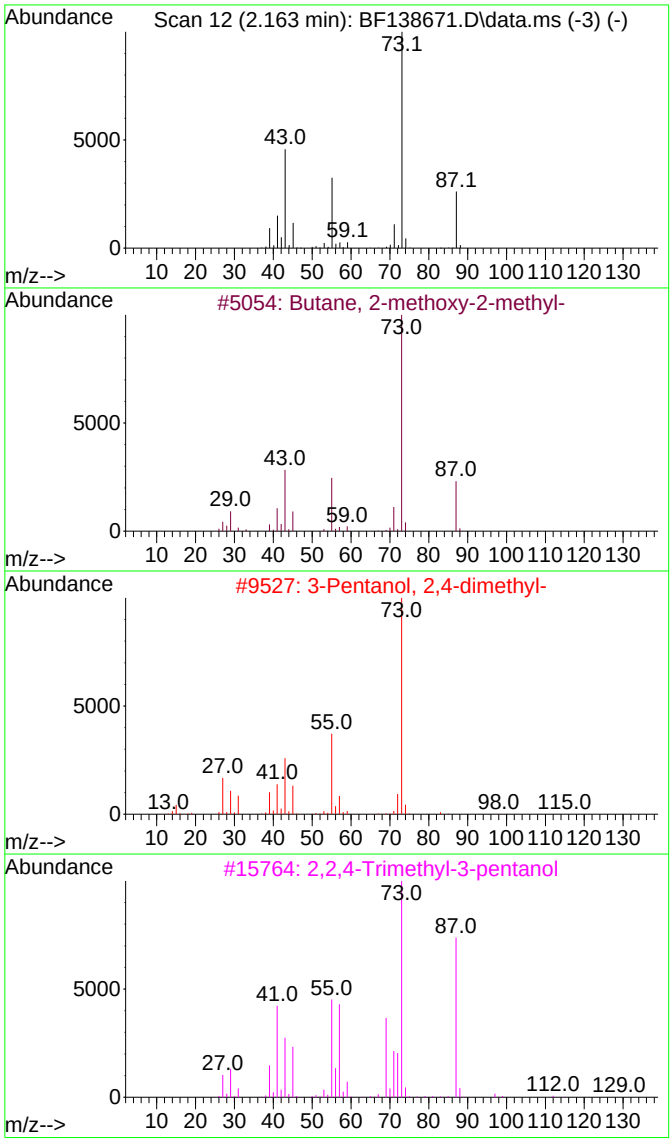
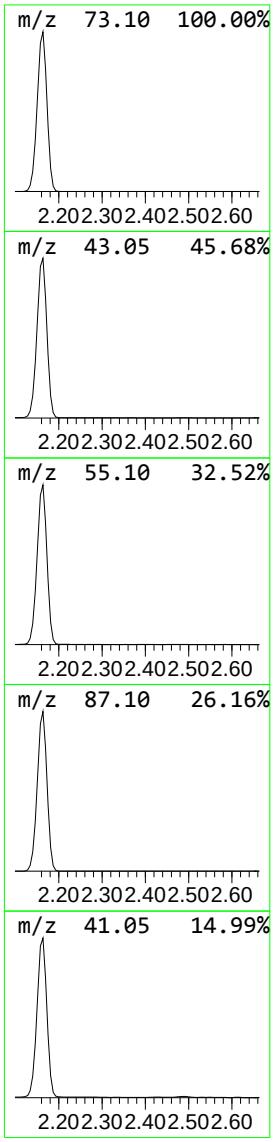
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	78.33 ng	2477540	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





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Data File : BF138671.D
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Operator : RC/JU
Sample : P3393-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-852-GI-SO-9.5-10-072624

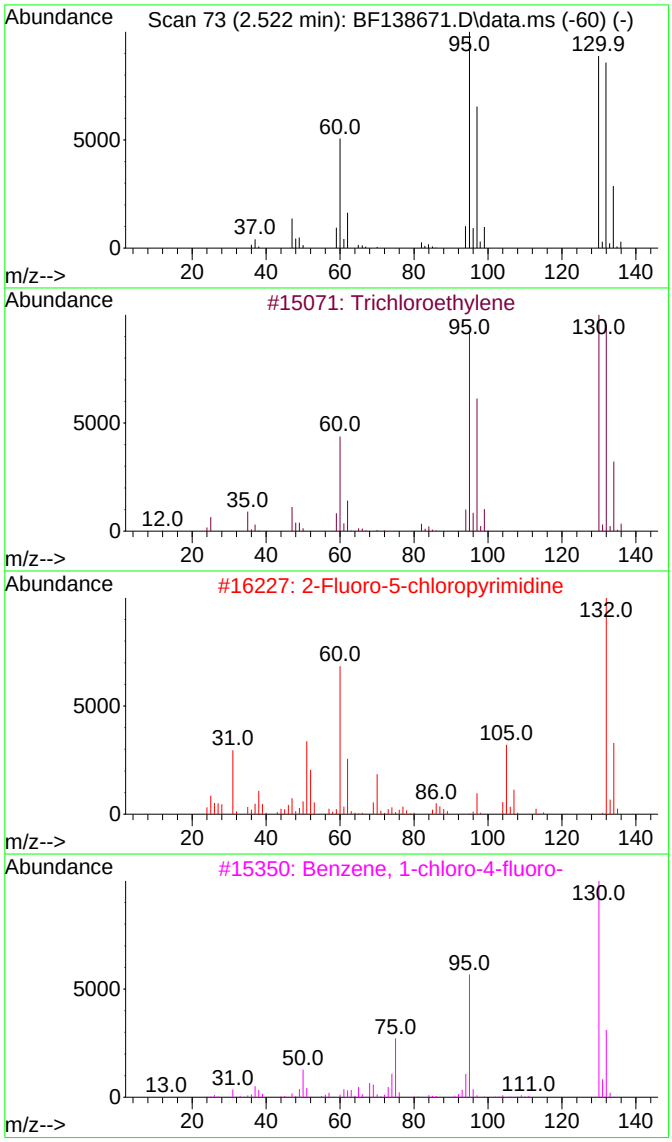
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

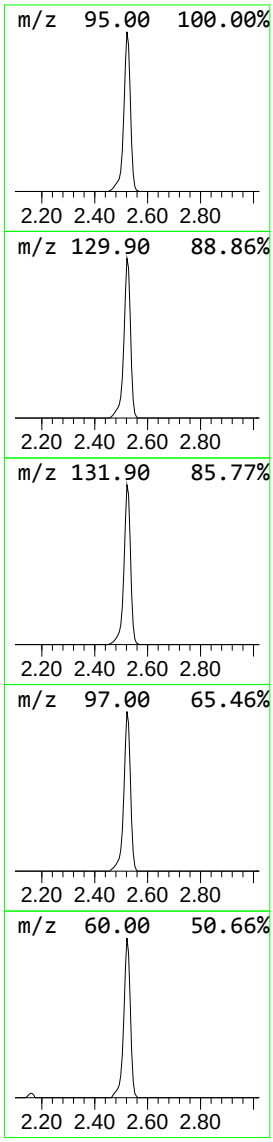
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Trichloroethylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.522	10.62 ng	335779	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroethylene	130	C2HCl3	000079-01-6	98
2	2-Fluoro-5-chloropyrimidine	132	C4H2ClFN2	062802-37-3	35
3	Benzene, 1-chloro-4-fluoro-	130	C6H4ClF	000352-33-0	22
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	22
5	1H-1,2,4-Triazol-3-amine, 5-(met...	130	C3H6N4S	045534-08-5	12





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Acq On : 29 Jul 2024 16:11
Operator : RC/JU
Sample : P3393-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-852-GI-SO-9.5-10-072624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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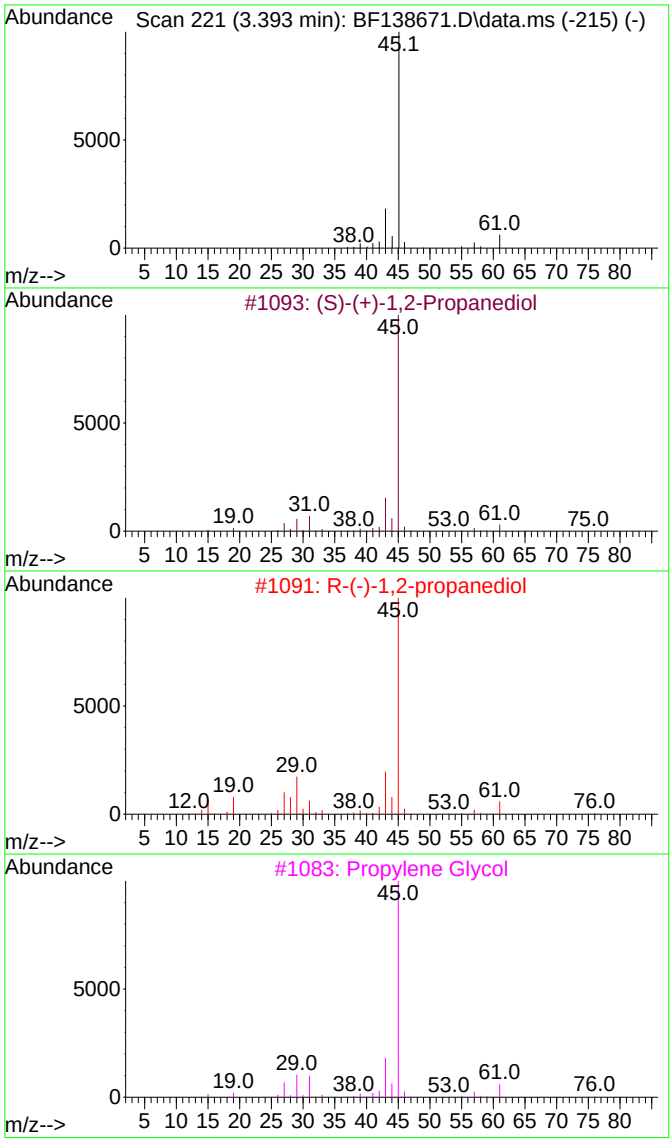
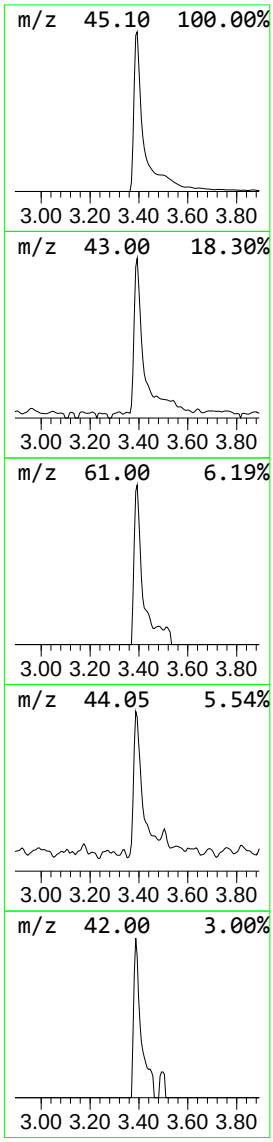
****

Peak Number 3 (S)-(+)-1,2-Propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.393	3.87 ng	122463	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	2-Butanol	74	C4H10O	000078-92-2	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9





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Data File : BF138671.D
Acq On : 29 Jul 2024 16:11
Operator : RC/JU
Sample : P3393-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-852-GI-SO-9.5-10-072624

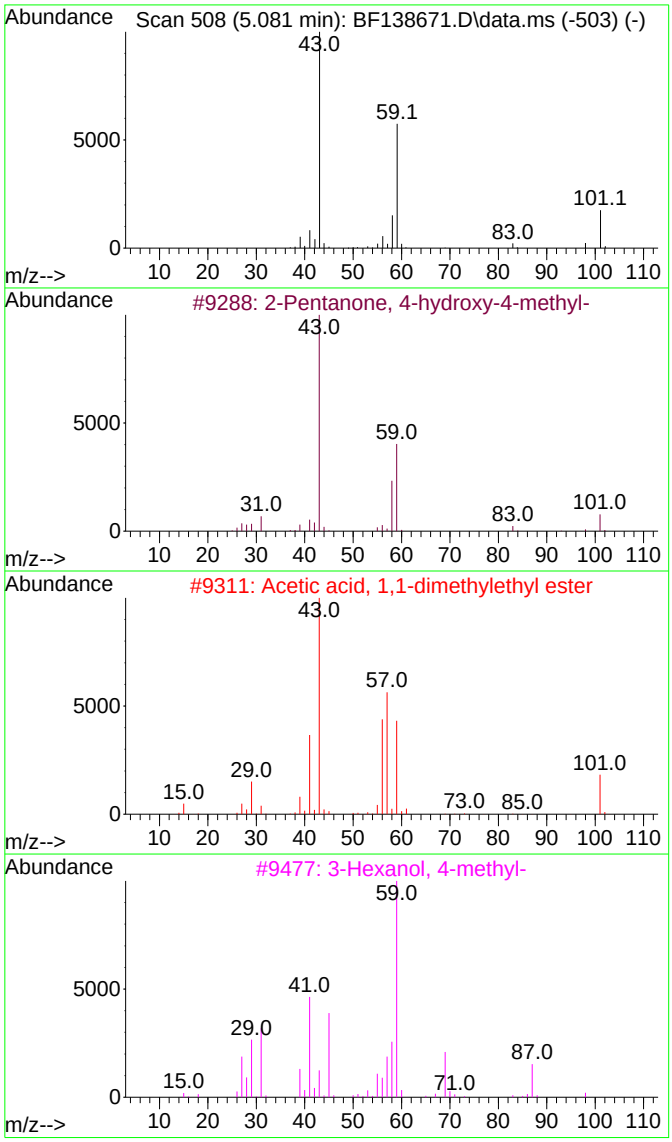
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

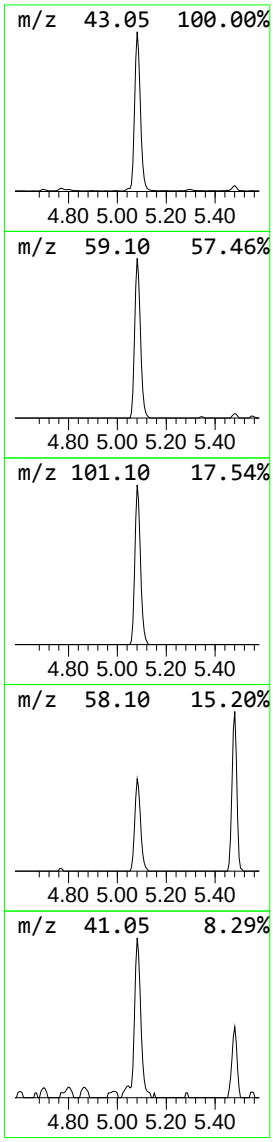
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	7.18 ng	227059	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072924\
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Operator : RC/JU
Sample : P3393-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-852-GI-SO-9.5-10-072624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

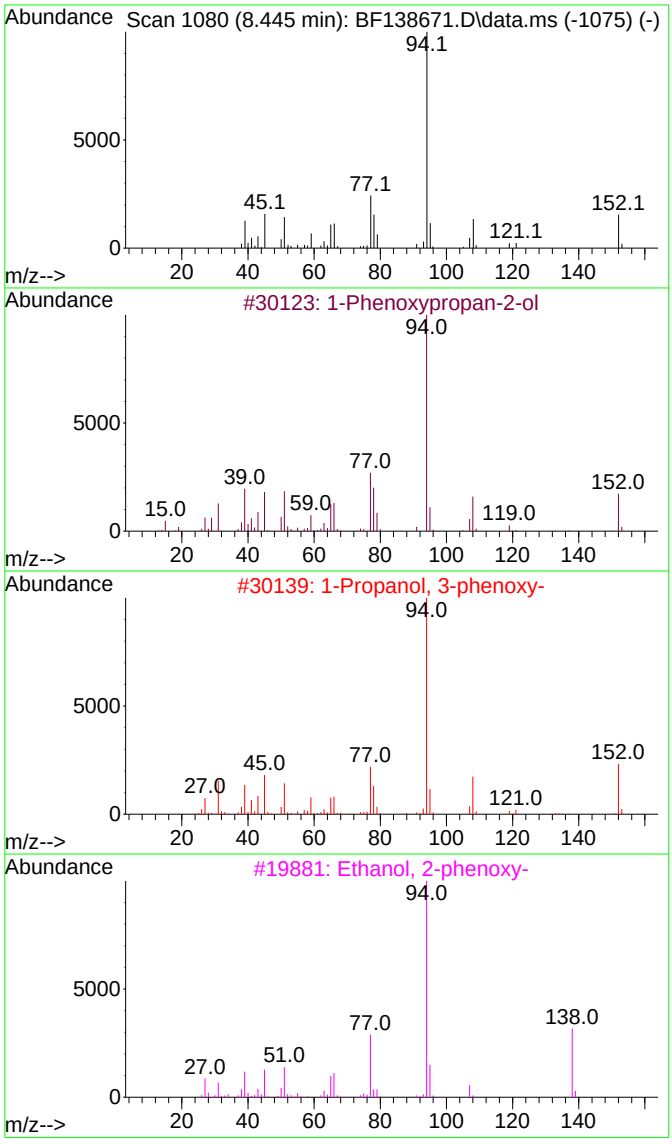
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

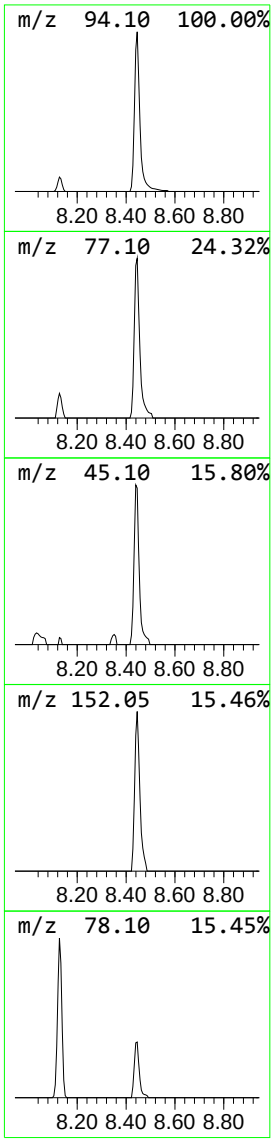
****

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.445	3.27 ng	133184	Naphthalene-d8	8.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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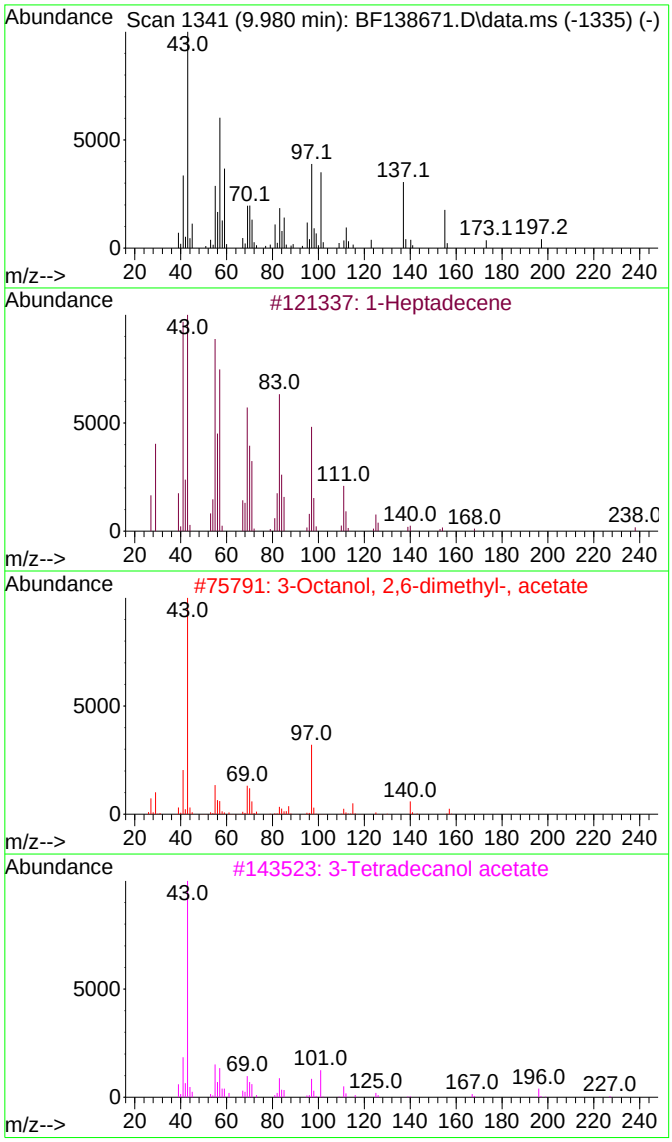
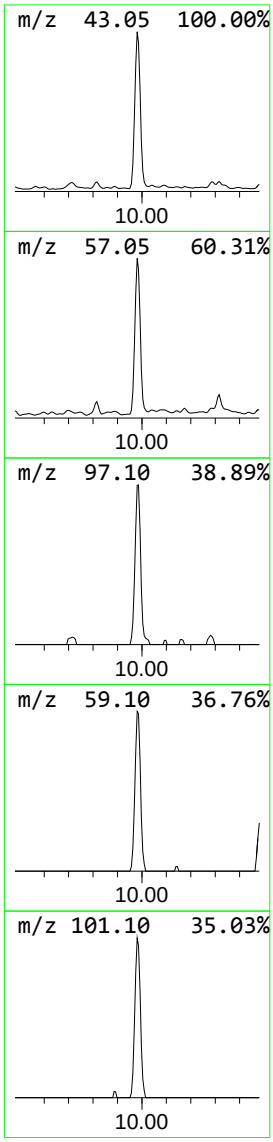
****

Peak Number 6 unknown9.980 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.980	3.76 ng	155653	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptadecene	238	C17H34	006765-39-5	27
2	3-Octanol, 2,6-dimethyl-, acetate	200	C12H24O2	123232-57-5	27
3	3-Tetradecanol acetate	256	C16H32O2	051354-23-5	25
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	22
5	9-Acetoxynonanal	200	C11H20O3	029541-97-7	22





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Sample : P3393-11
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-852-GI-SO-9.5-10-072624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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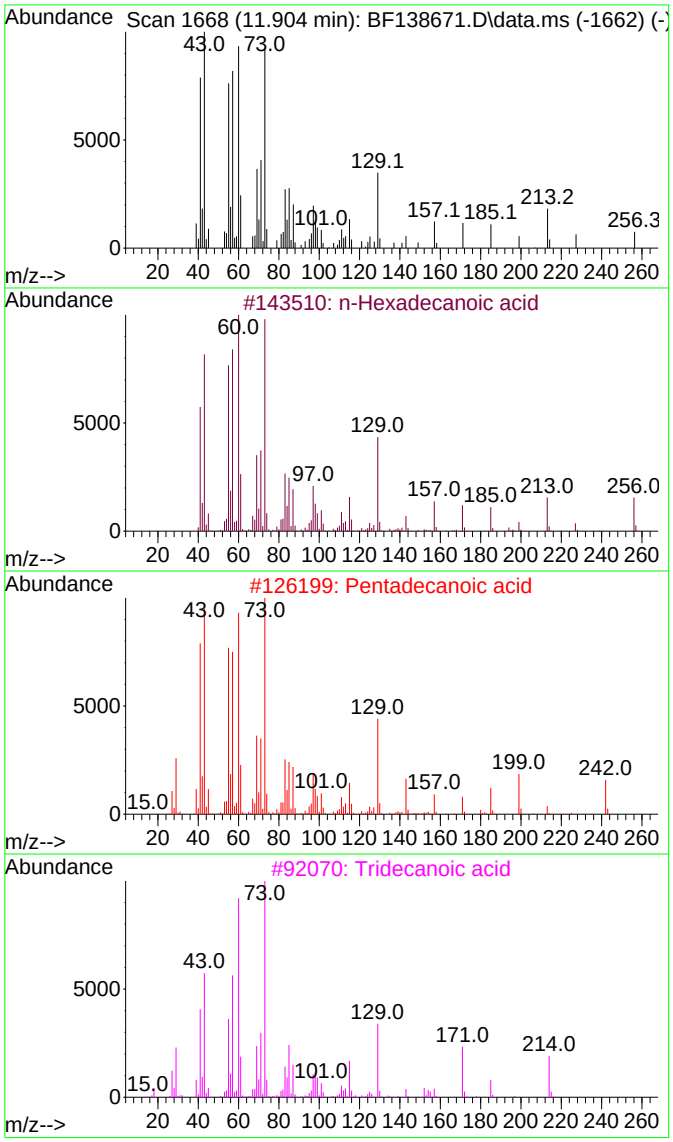
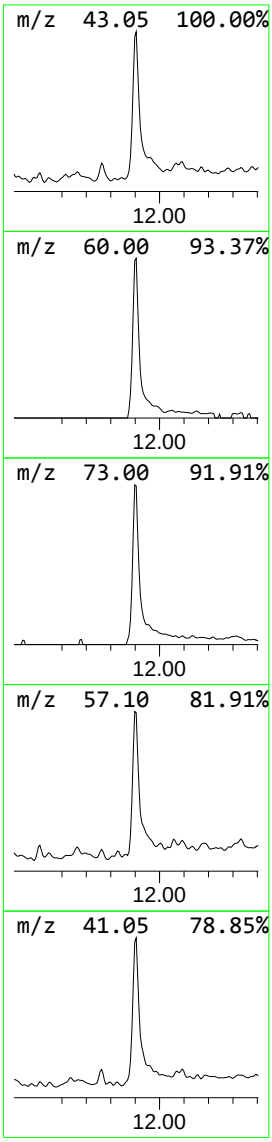
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	4.93 ng	163364	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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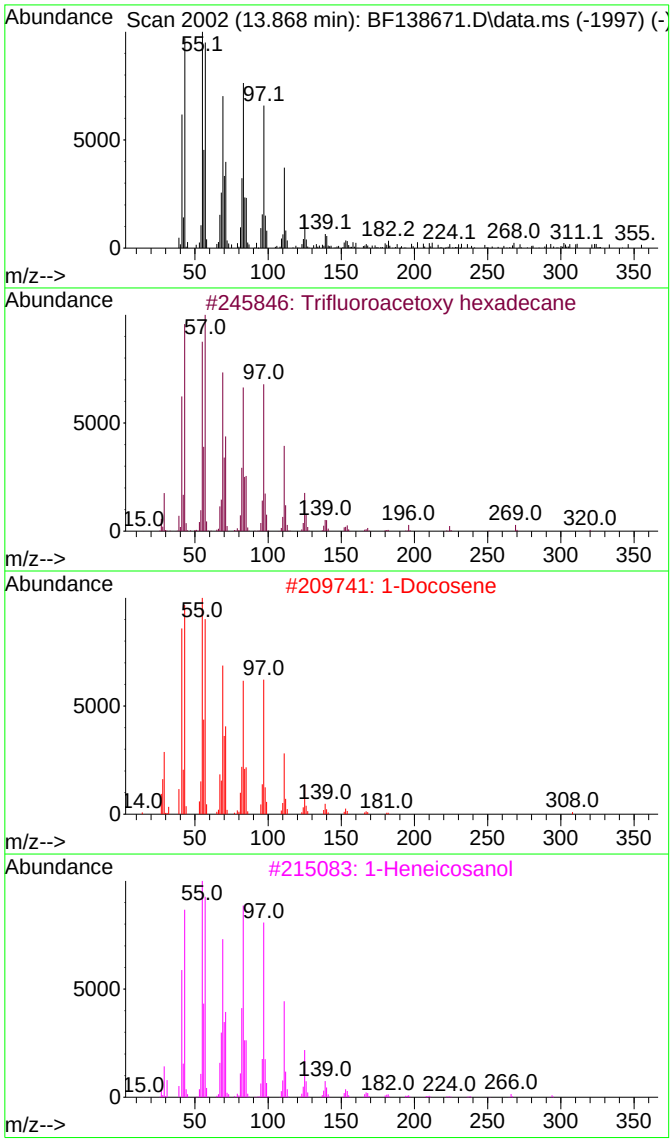
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

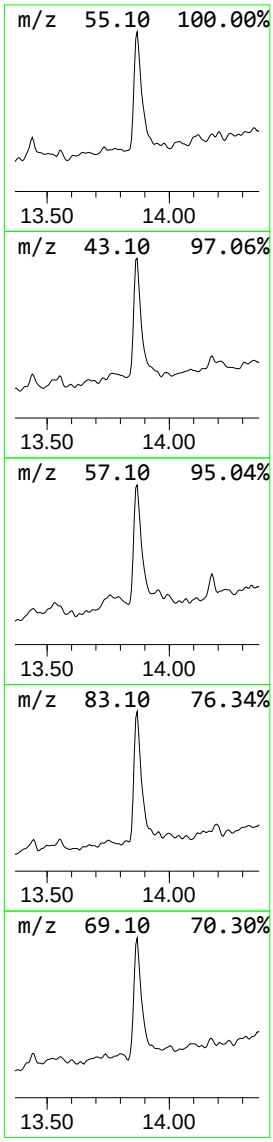
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	9.64 ng	251325	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
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...	2.163	78.3	ng	2477540	1	6.851	632572	20.0
Trichloroethylene	2.522	10.6	ng	335779	1	6.851	632572	20.0
(S)-(+)-1,2-Pro...	3.393	3.9	ng	122463	1	6.851	632572	20.0
2-Pentanone, 4-...	5.081	7.2	ng	227059	1	6.851	632572	20.0
1-Phenoxypropan...	8.445	3.3	ng	133184	2	8.128	813572	20.0
unknown9.980	9.980	3.8	ng	155653	3	9.886	828610	20.0
n-Hexadecanoic ...	11.904	4.9	ng	163364	4	11.374	662448	20.0
Trifluoroacetox...	13.868	9.6	ng	251325	5	14.015	521379	20.0