LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082319\
Data File : BF116490.D
Acq On : 23 Aug 2019 21:12
Operator : HP/JU
Sample : K4330-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0649-ELUTRIATE-COMP-C

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-BF082319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	12	22	26	rVB	5516108	8485617	52.67%	16.115%
2	5.498	575	580	584	rBV	1649354	1485163	9.22%	2.820%
3	5.545	584	588	601	rVB	286524	615429	3.82%	1.169%
4	6.492	745	749	763	rBV	296641	408184	2.53%	0.775%
5	6.651	771	776	779	rBV	1652317	1709724	10.61%	3.247%
6	6.692	779	783	811	rVB2	807227	2964442	18.40%	5.630%
7	6.881	811	815	819	rBV	916360	733699	4.55%	1.393%
8	7.039	838	842	845	rBV	3093778	2688467	16.69%	5.106%
9	7.439	904	910	913	rBV	2250775	2088900	12.97%	3.967%
10	7.616	930	940	942	rBV	8014032	16109741	100.00%	30.594%
11	8.063	1012	1016	1020	rBV	689764	616794	3.83%	1.171%
12	8.163	1029	1033	1037	rVB	1080755	903529	5.61%	1.716%
13	8.434	1076	1079	1082	rVB	300078	229128	1.42%	0.435%
14	9.122	1192	1196	1204	rBV	169207	168231	1.04%	0.319%
15	9.233	1210	1215	1219	rBV	3839042	3855435	23.93%	7.322%
16	9.622	1278	1281	1284	rBV	264480	204006	1.27%	0.387%
17	9.910	1326	1330	1334	rVB	1150435	1000125	6.21%	1.899%
18	10.698	1459	1464	1467	rBV	2236302	2021429	12.55%	3.839%
19	11.392	1578	1582	1586	rBV	1111788	894251	5.55%	1.698%
20	11.922	1667	1672	1679	rBV	445921	467494	2.90%	0.888%
21	12.710	1802	1806	1818	rBV	236876	290859	1.81%	0.552%
22	12.980	1847	1852	1855	rBV	3343317	3021613	18.76%	5.738%
23	13.874	2000	2004	2014	rBV	365149	357321	2.22%	0.679%
24	14.021	2024	2029	2033	rBV2	710251	729820	4.53%	1.386%
25	15.486	2273	2278	2283	rBV	506220	606962	3.77%	1.153%

Sum of corrected areas: 52656363

LSC Report - Integrated Chromatogram

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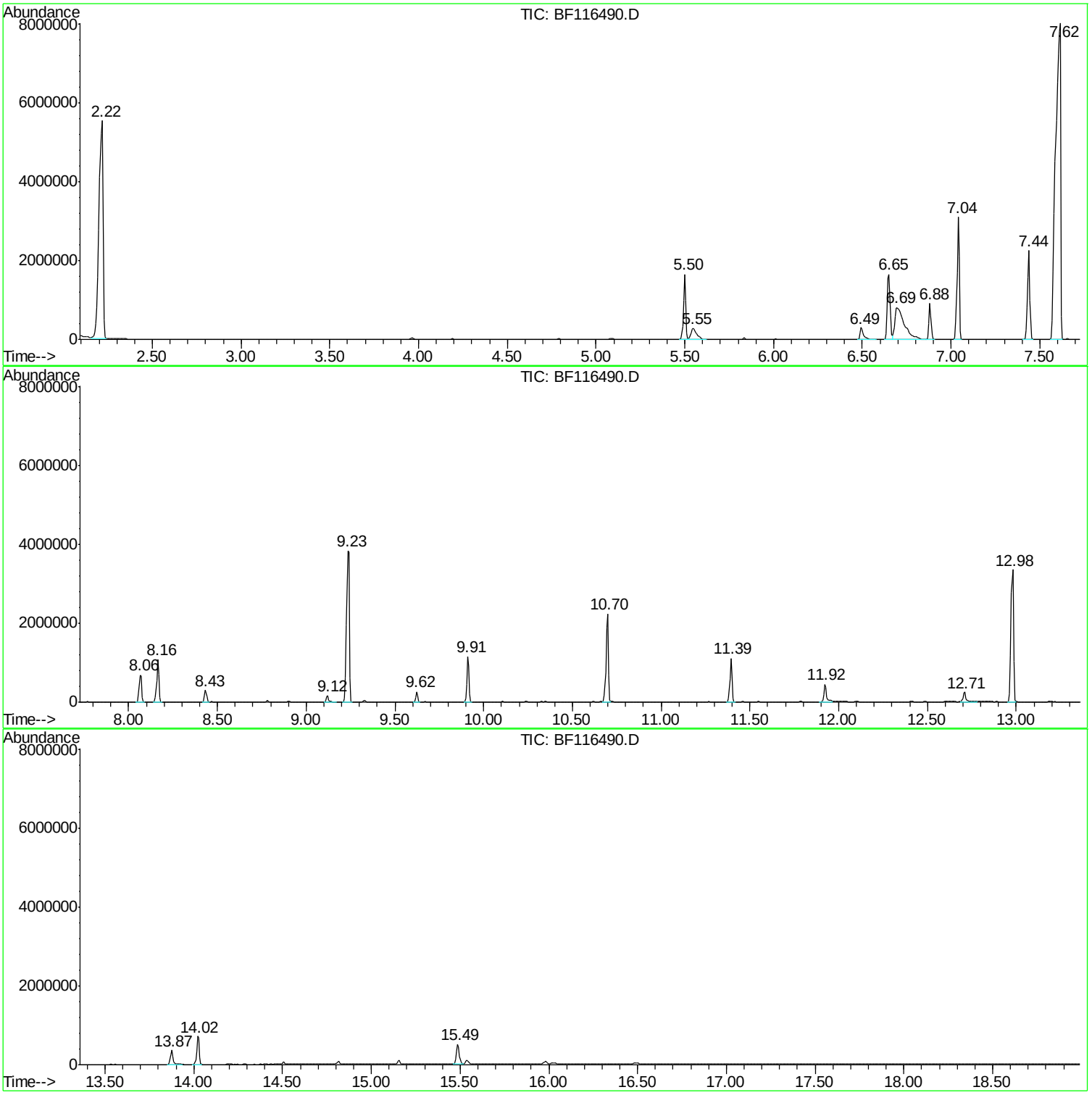
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0649-ELUTRIATE-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082319\
Data File : BF116490.D
Acq On : 23 Aug 2019 21:12
Operator : HP/JU
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0649-ELUTRIATE-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

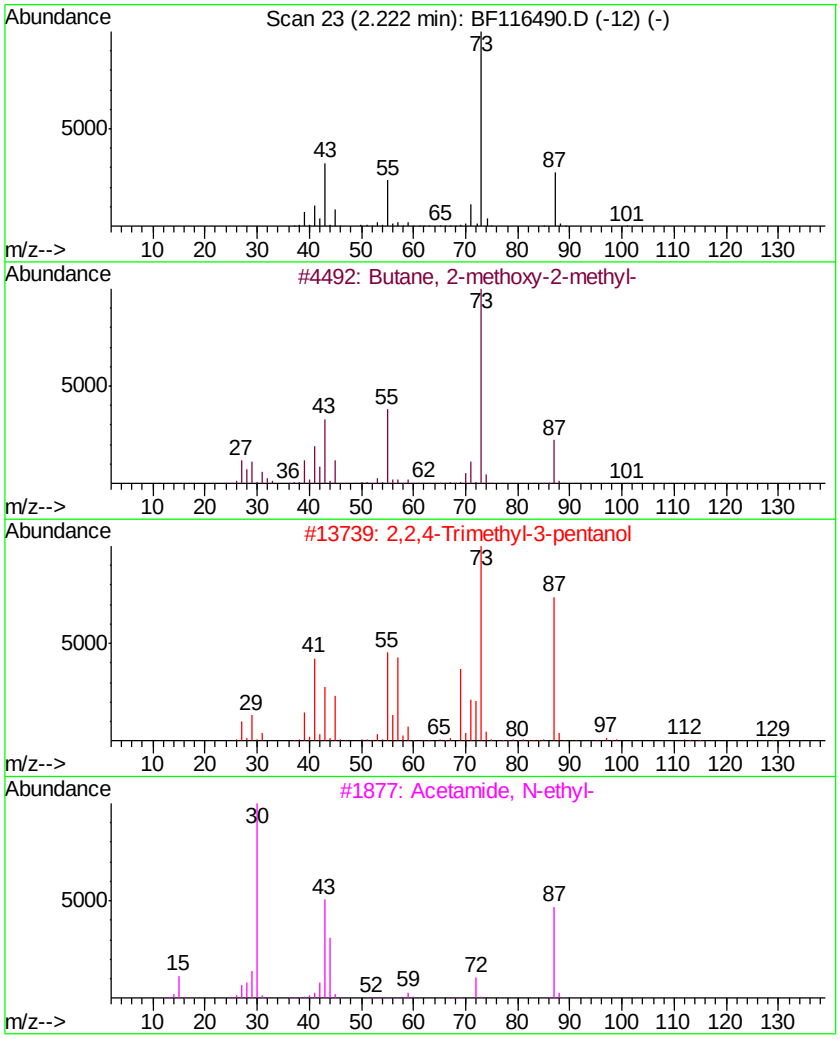
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

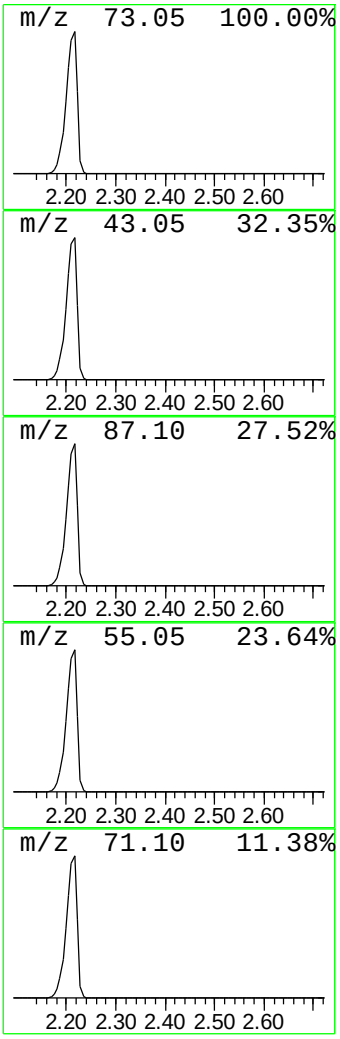
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	231.31 ng	8485620	1,4-Dichlorobenzene-d4	6.88

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Library Search Compound Report

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Acq On : 23 Aug 2019 21:12
Operator : HP/JU
Sample : K4330-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0649-ELUTRIATE-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

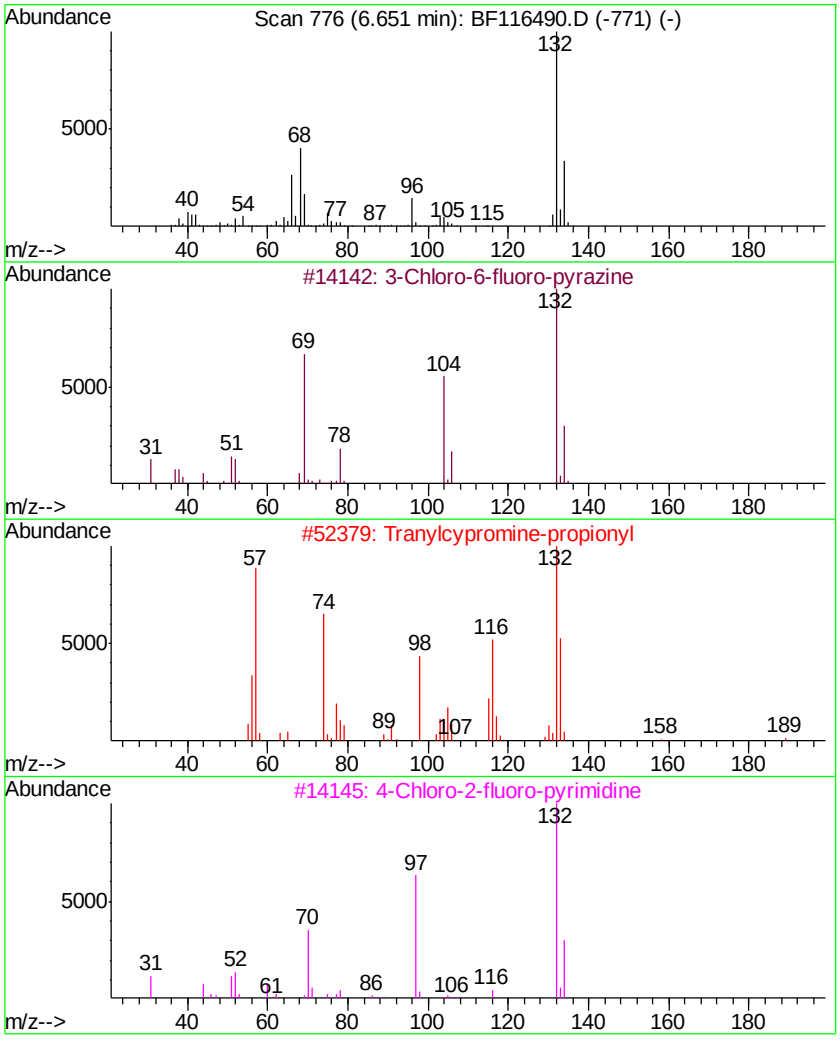
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

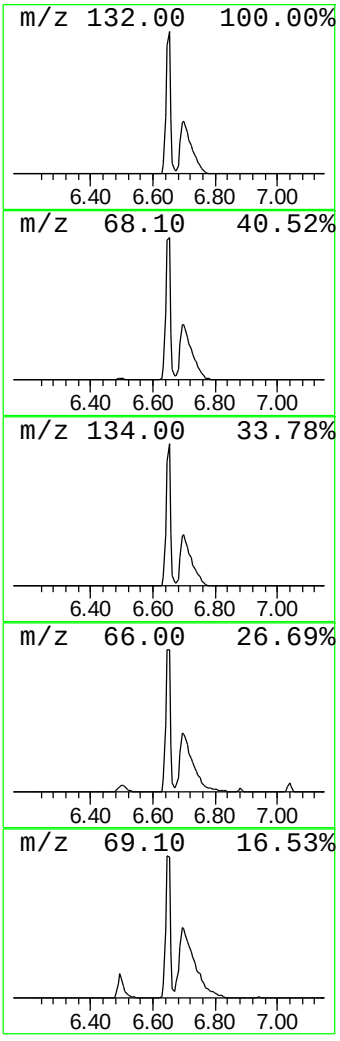
****

Peak Number 2 unknown6.65 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	46.61 ng	1709720	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





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Data File : BF116490.D
Acq On : 23 Aug 2019 21:12
Operator : HP/JU
Sample : K4330-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0649-ELUTRIATE-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

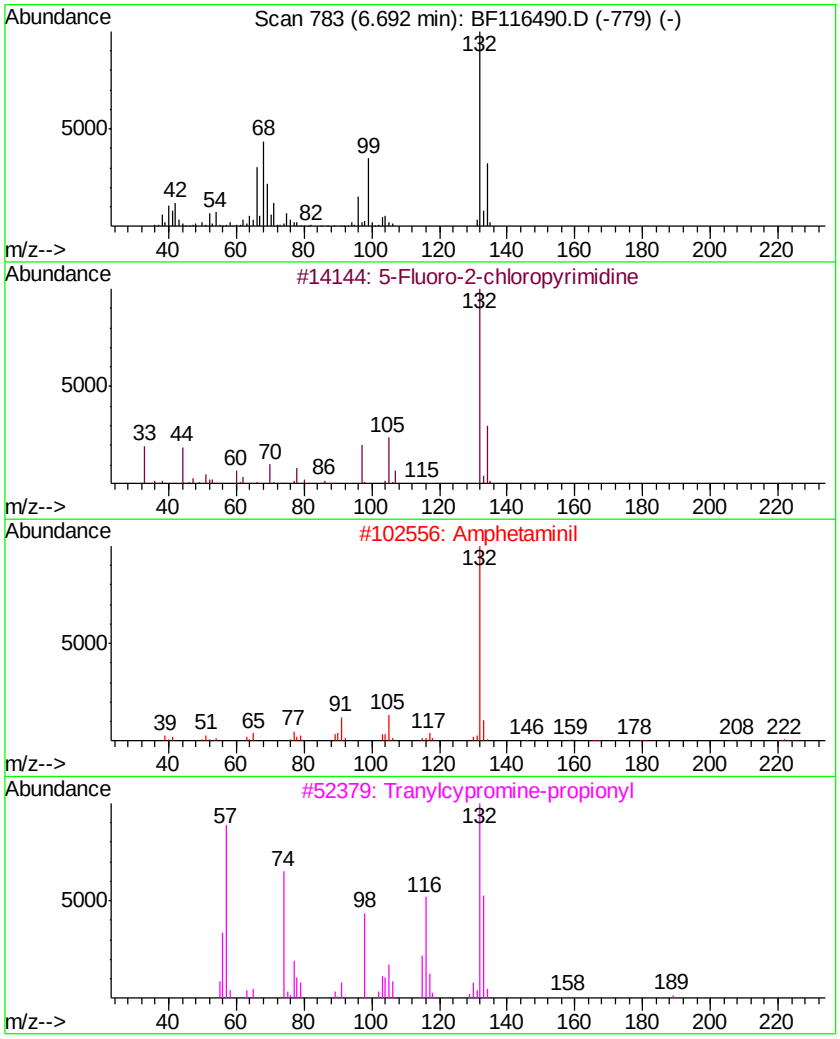
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

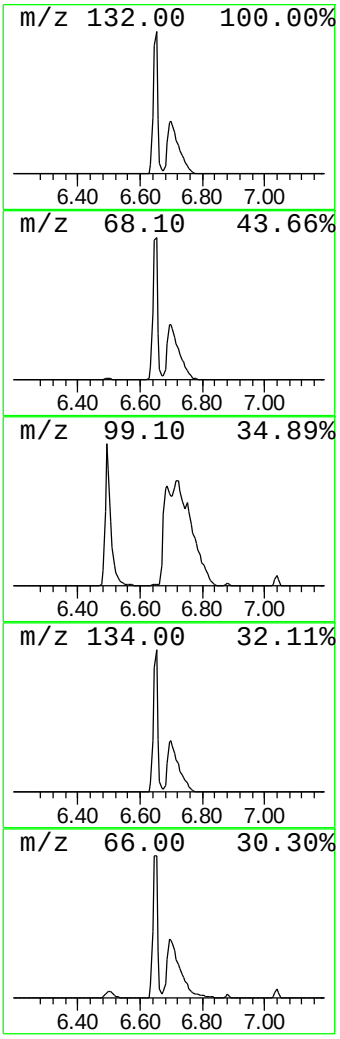
****

Peak Number 3 unknown6.69 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	80.81 ng	2964440	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	Amphetaminil	250	C17H18N2	017590-01-1	10
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Data File : BF116490.D
Acq On : 23 Aug 2019 21:12
Operator : HP/JU
Sample : K4330-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0649-ELUTRIATE-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

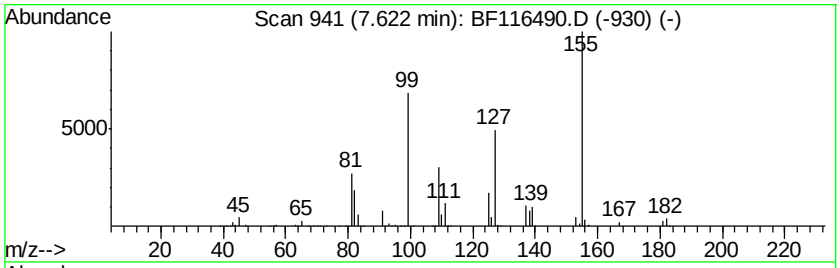
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

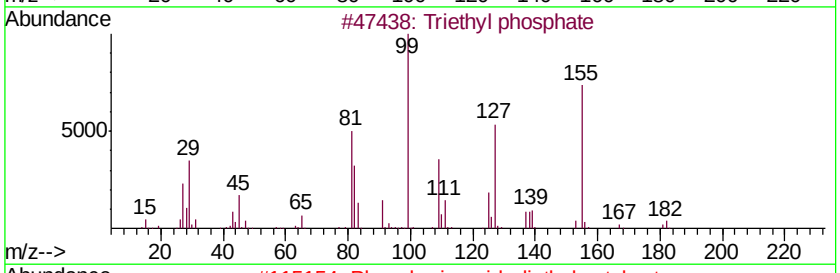
****

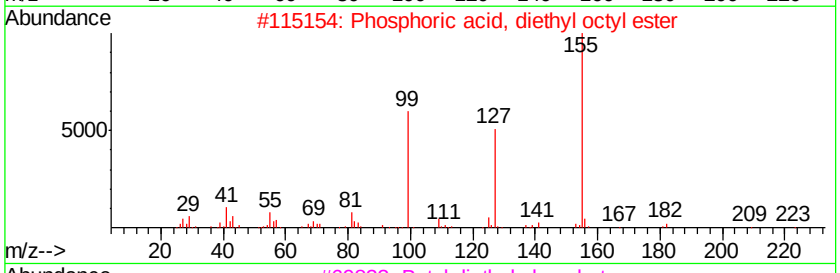
Peak Number 5 Triethyl phosphate Concentration Rank 1

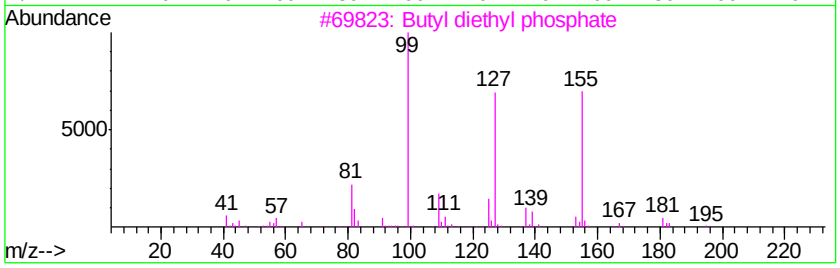
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.62	356.60 ng	16109700	Naphthalene-d8	8.16

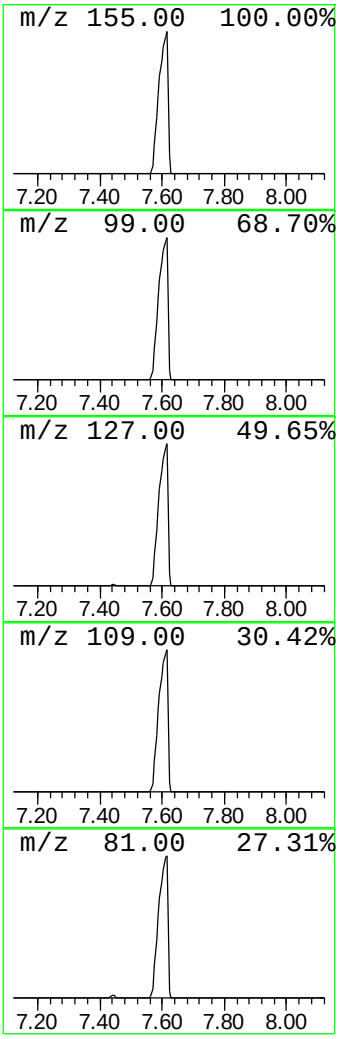
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl phosphate	182	C6H15O4P	000078-40-0	96
2	Phosphoric acid, diethyl octyl e...	266	C12H27O4P	1000308-90-4	50
3	Butyl diethyl phosphate	210	C8H19O4P	1000298-58-0	39
4	Diethyl isopropylidenemalonate	200	C10H16O4	006802-75-1	36
5	Phosphoric acid, diethyl pentyl ...	224	C9H21O4P	020195-08-8	36











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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0649-ELUTRIATE-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

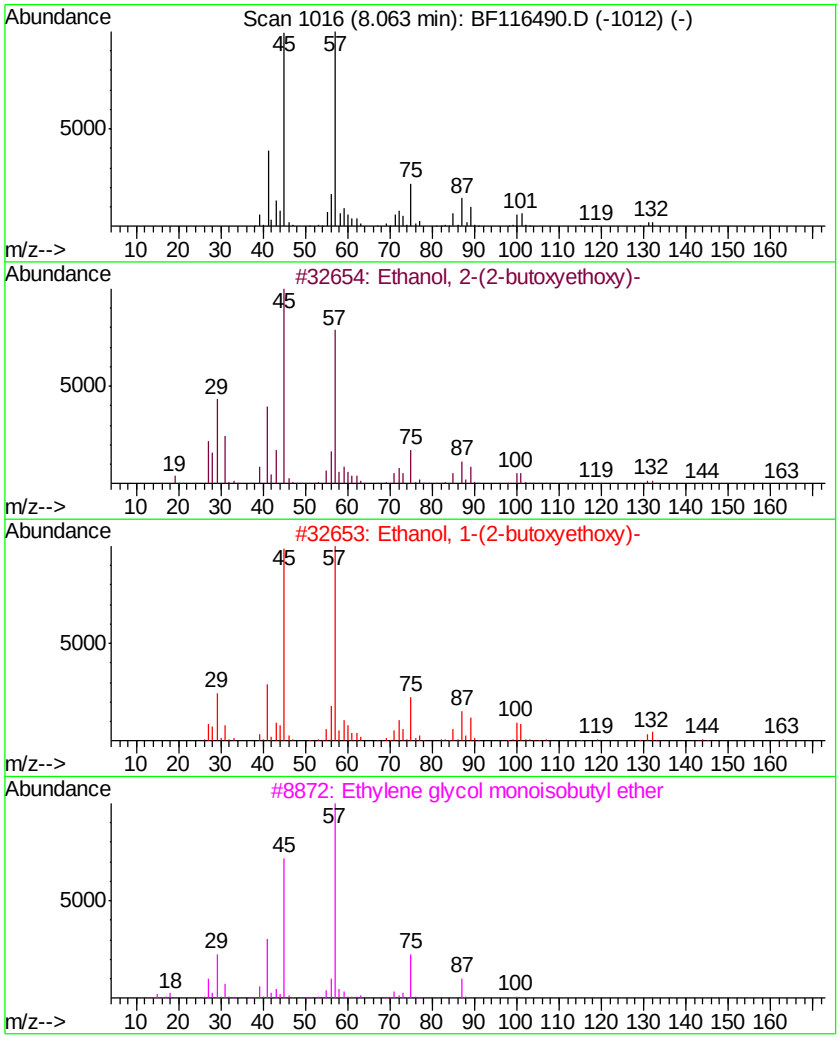
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

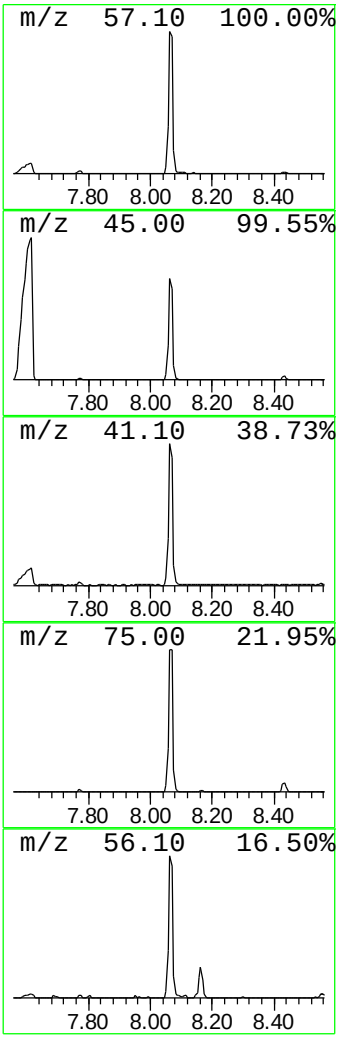
****

Peak Number 6 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.06	13.65 ng	616794	Naphthalene-d8	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Di-sec-butyl ether	130	C8H18O	006863-58-7	50
5	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50





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Sample : K4330-05
Misc :
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Instrument : BNA_F
ClientSampleId : 0649-ELUTRIATE-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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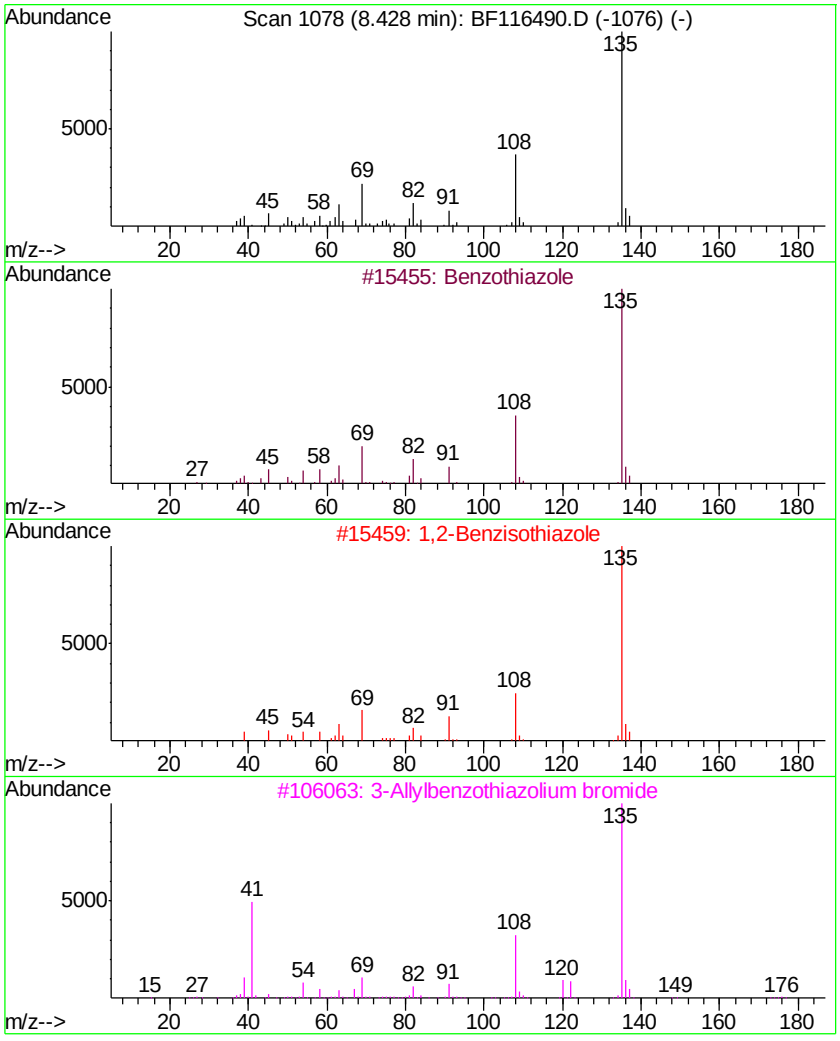
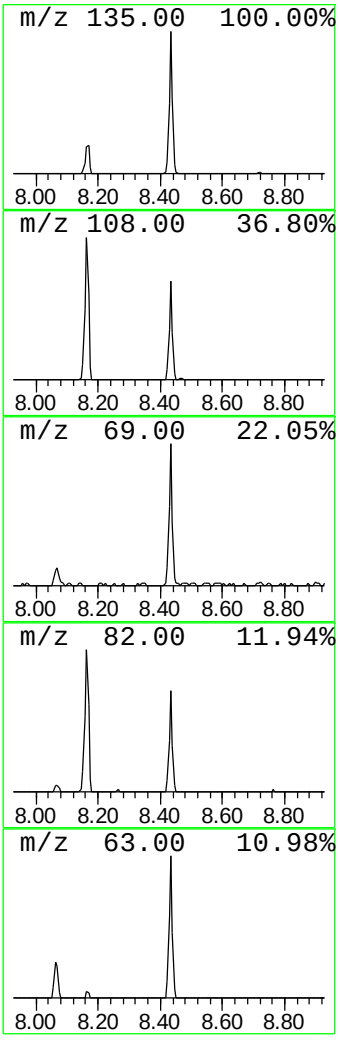
Peak Number 7 Benzothiazole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.43	5.07 ng	229128	Naphthalene-d8	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	97
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	90
3	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	78
4	1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	64
5	Adenine	135	C5H5N5	000073-24-5	59





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Misc :
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Instrument : BNA_F
ClientSampleId : 0649-ELUTRIATE-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
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TIC Library : C:\DATABASE\NIST11.L
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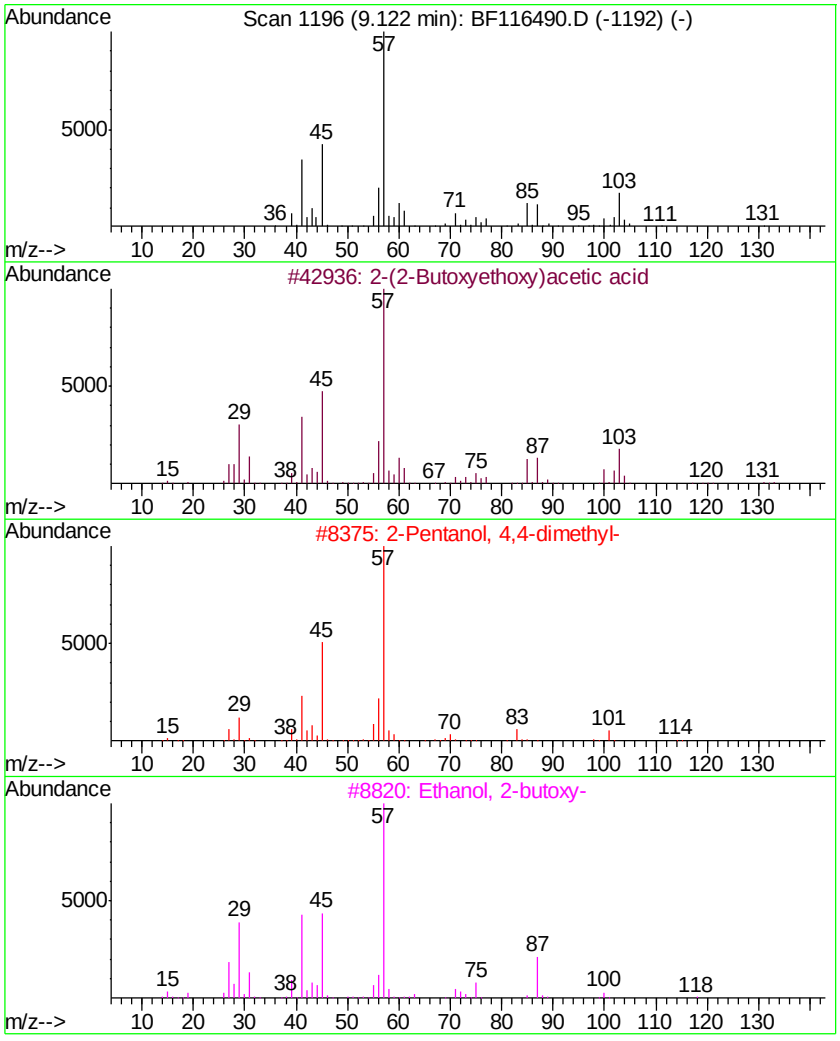
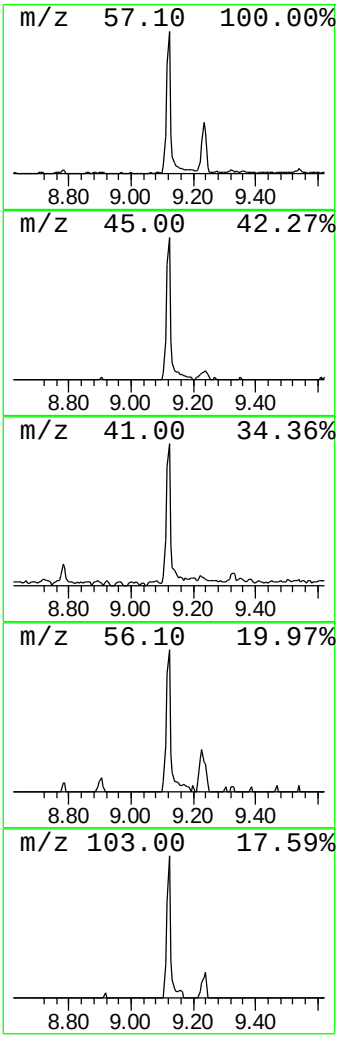
Peak Number 8 2-(2-Butoxyethoxy)acetic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.12	3.36 ng	168231	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Butoxyethoxy)acetic acid	176	C8H16O4	082941-26-2	72
2	2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	47
3	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	47
4	Butane, 1-(2-methoxyethoxy)-	132	C7H16O2	013343-98-1	38
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	38





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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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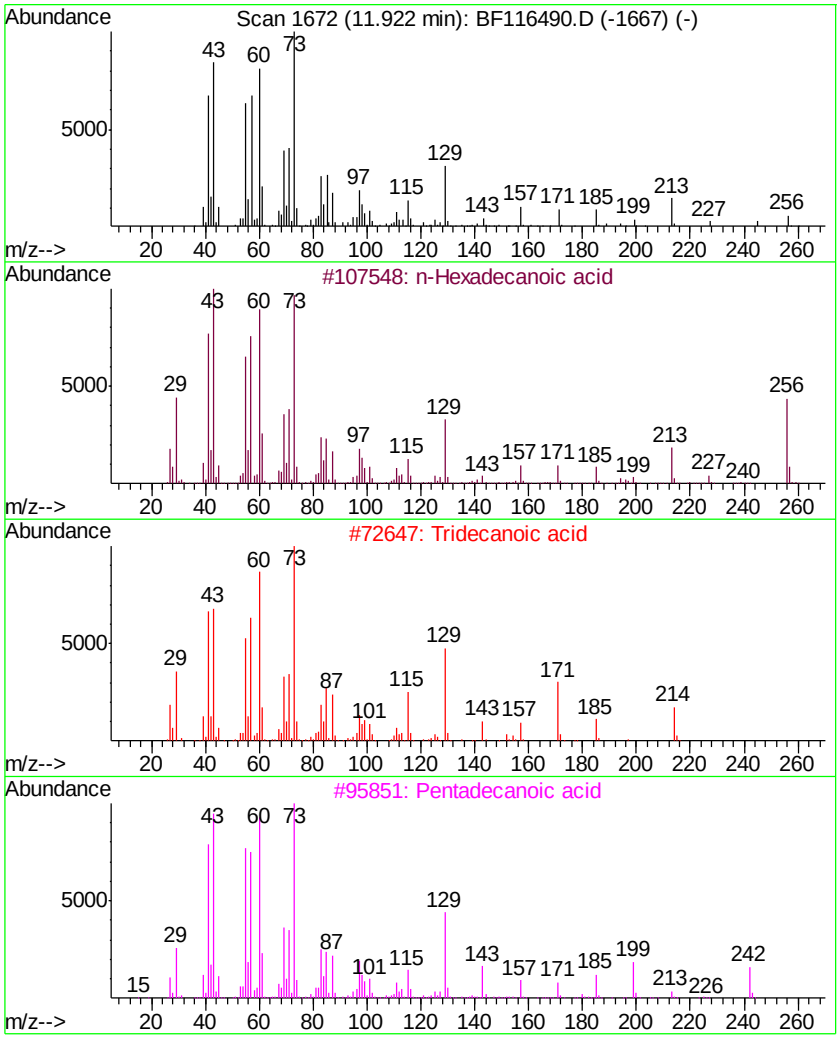
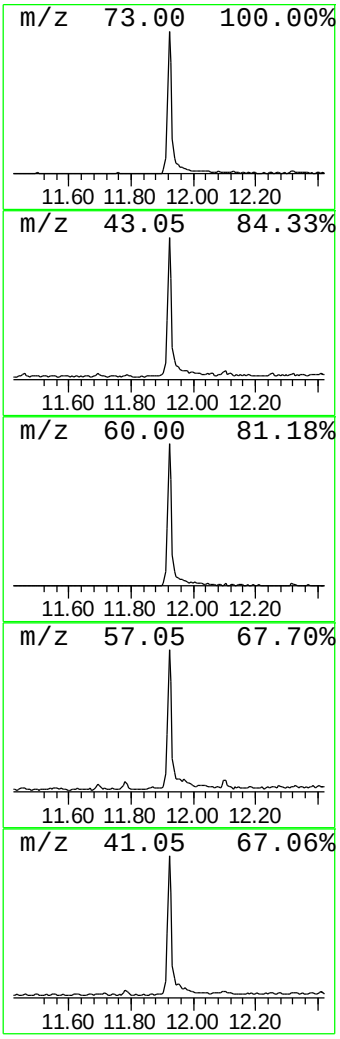
Peak Number 9 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	10.46 ng	467494	Phenanthrene-d10	11.39

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20
5	Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	18





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Data File : BF116490.D
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Sample : K4330-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0649-ELUTRIATE-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

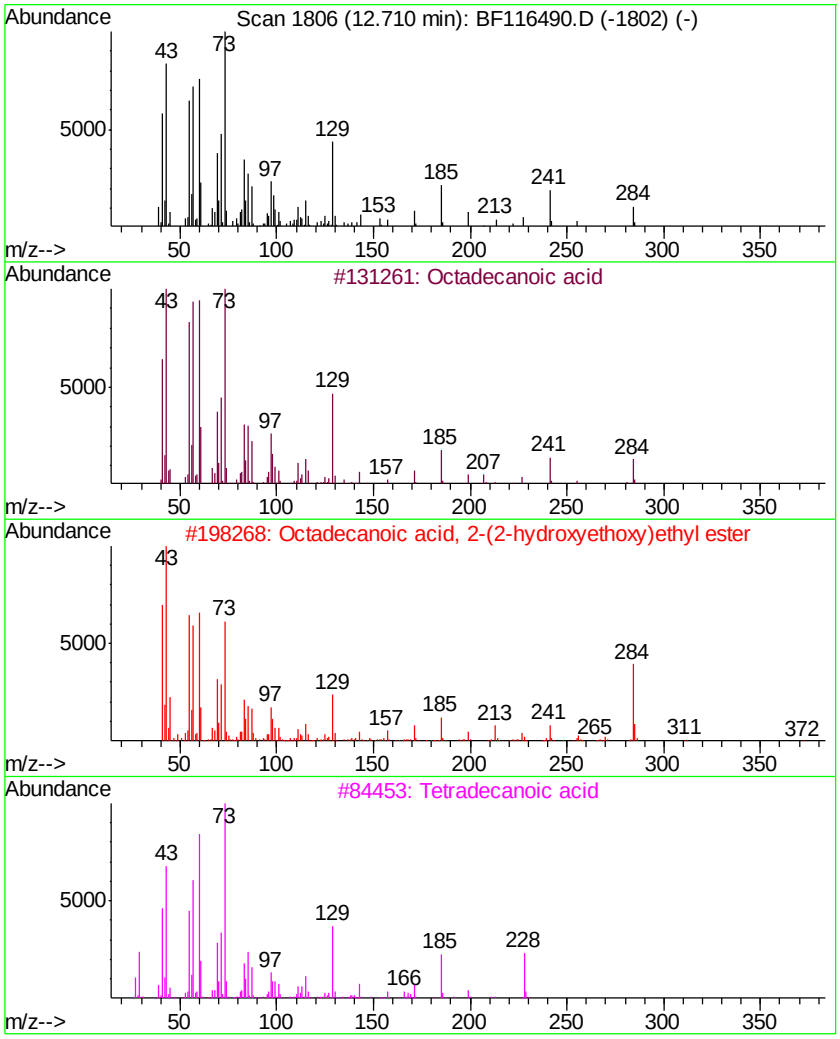
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

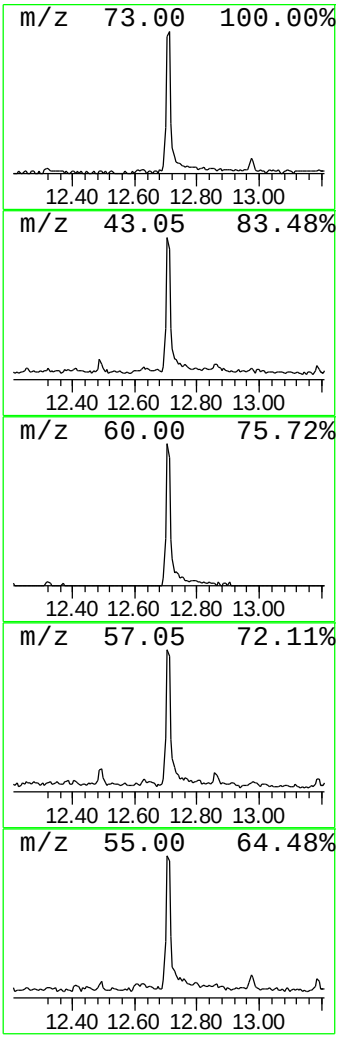
****

Peak Number 10 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	7.97 ng	290859	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	53





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082319\
Data File : BF116490.D
Acq On : 23 Aug 2019 21:12
Operator : HP/JU
Sample : K4330-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
0649-ELUTRIATE-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

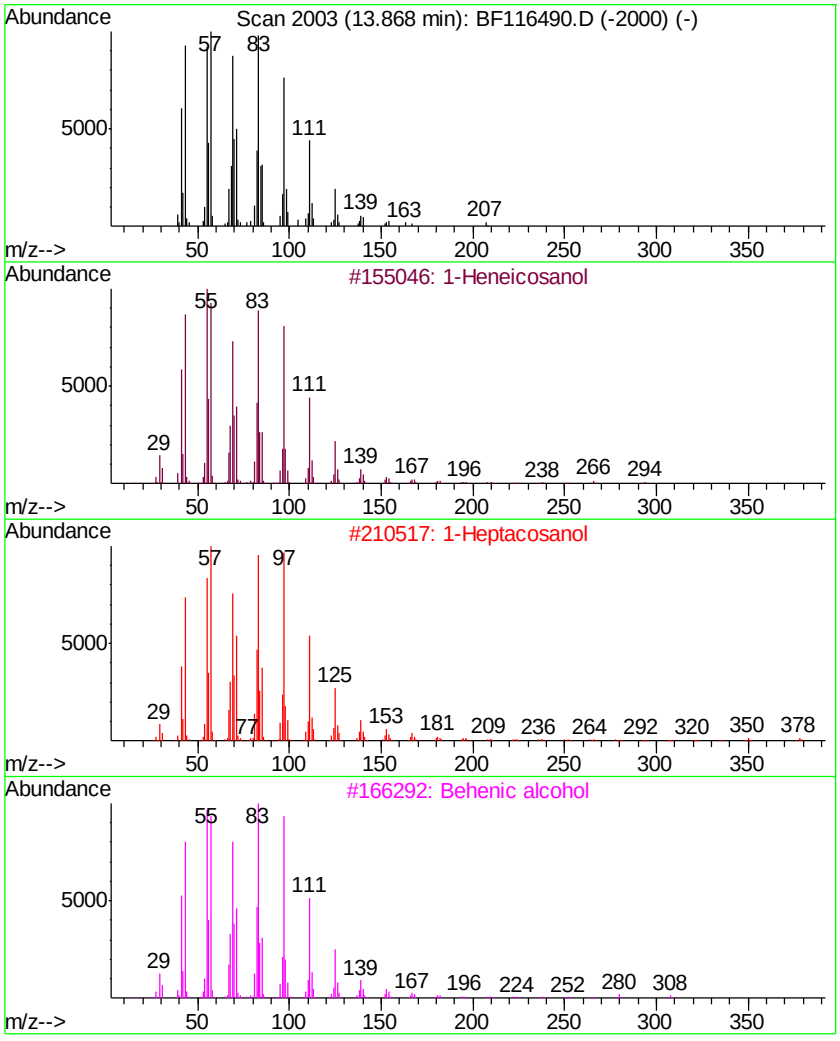
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

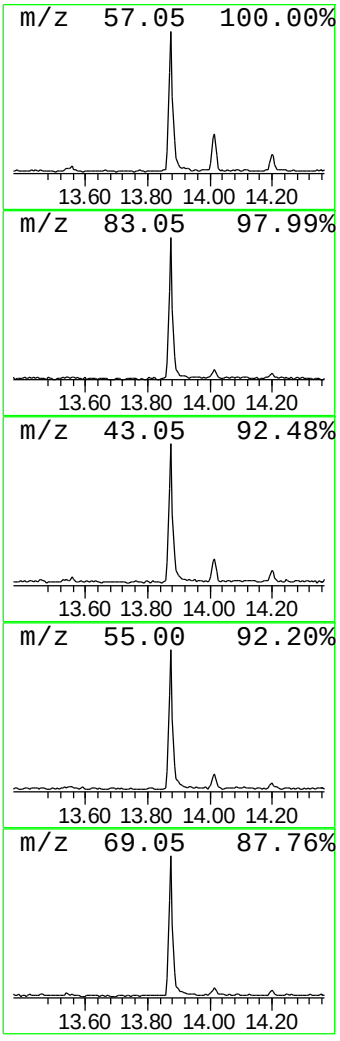
****

Peak Number 11 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	9.79 ng	357321	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	1-Heptacosanol	396	C27H56O	002004-39-9	93
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082319\
Data File : BF116490.D
Acq On : 23 Aug 2019 21:12
Operator : HP/JU
Sample : K4330-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 0649-ELUTRIATE-COMP-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.22	231.3	ng	8485620	1	6.88	733699	20.0
unknown6.65	6.65	46.6	ng	1709720	1	6.88	733699	20.0
unknown6.69	6.69	80.8	ng	2964440	1	6.88	733699	20.0
Triethyl phosphate	7.62	356.6	ng	16109700	2	8.16	903529	20.0
Ethanol, 2-(2-but...	8.06	13.7	ng	616794	2	8.16	903529	20.0
Benzothiazole	8.43	5.1	ng	229128	2	8.16	903529	20.0
2-(2-Butoxyethoxy...	9.12	3.4	ng	168231	3	9.91	1000130	20.0
n-Hexadecanoic acid	11.92	10.5	ng	467494	4	11.39	894251	20.0
Octadecanoic acid	12.71	8.0	ng	290859	5	14.03	729820	20.0
1-Heneicosanol	13.87	9.8	ng	357321	5	14.03	729820	20.0