LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100424\
Data File : BF139663.D
Acq On : 04 Oct 2024 17:55
Operator : RC/JU
Sample : P4254-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-147

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-BF100124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139663.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	18	rVB	4648123	8070731	100.00%	22.862%
2	5.481	571	576	593	rBV	918532	1208003	14.97%	3.422%
3	6.163	687	692	707	rBV	148728	192392	2.38%	0.545%
4	6.498	743	749	772	rBV	540747	838268	10.39%	2.375%
5	6.863	806	811	816	rBV	459236	557890	6.91%	1.580%
6	7.428	900	907	912	rBV	1132318	1543563	19.13%	4.373%
7	8.145	1023	1029	1037	rVB	578657	723754	8.97%	2.050%
8	8.375	1060	1068	1070	rBV	3490750	5990727	74.23%	16.970%
9	8.398	1070	1072	1081	rVV	3915729	4926516	61.04%	13.956%
10	8.475	1081	1085	1089	rVV	593314	807963	10.01%	2.289%
11	8.510	1089	1091	1103	rVB	157924	258253	3.20%	0.732%
12	9.222	1205	1212	1217	rBV	2111192	2707557	33.55%	7.670%
13	9.416	1234	1245	1251	rBV4	33122	92836	1.15%	0.263%
14	9.898	1322	1327	1332	rBV	643491	791500	9.81%	2.242%
15	10.610	1443	1448	1454	rBV	284478	358196	4.44%	1.015%
16	10.686	1455	1461	1470	rBV	1294102	1732075	21.46%	4.907%
17	11.386	1574	1580	1586	rBV	621319	806118	9.99%	2.284%
18	11.910	1664	1669	1690	rBV2	46752	132092	1.64%	0.374%
19	12.968	1843	1849	1854	rBV	1868433	2411620	29.88%	6.831%
20	14.021	2023	2028	2037	rVB	398205	515142	6.38%	1.459%
21	14.986	2187	2192	2199	rBV	70014	96667	1.20%	0.274%
22	15.492	2271	2278	2288	rBV	332498	539744	6.69%	1.529%

Sum of corrected areas: 35301607

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100424\
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Instrument :
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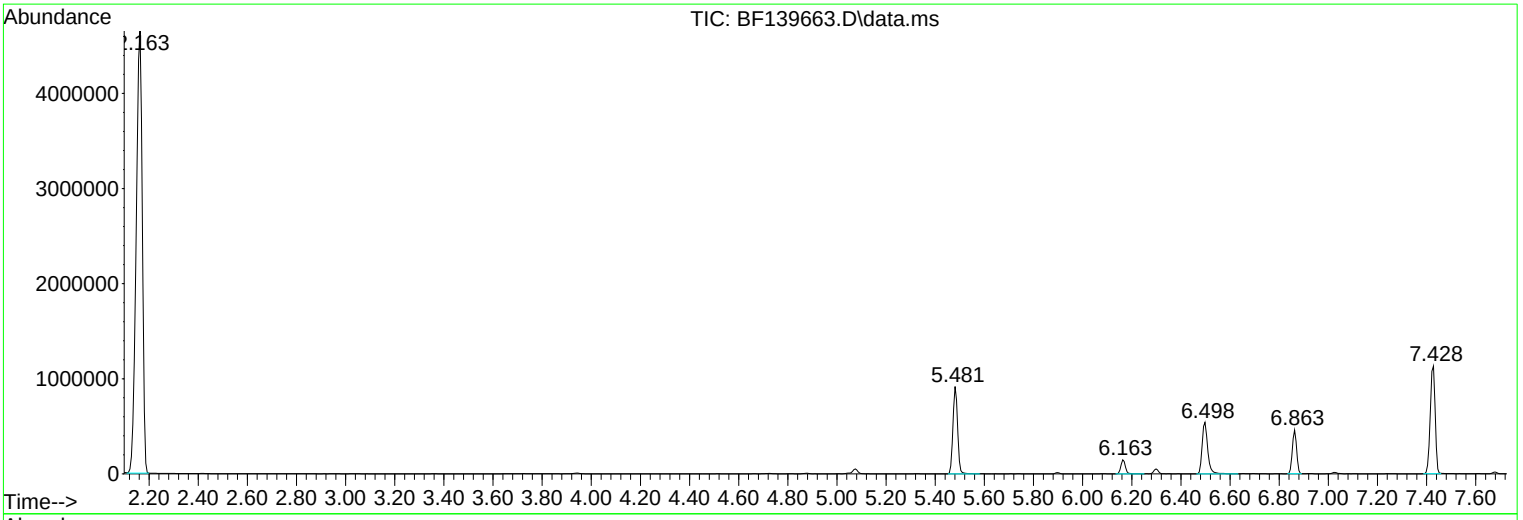
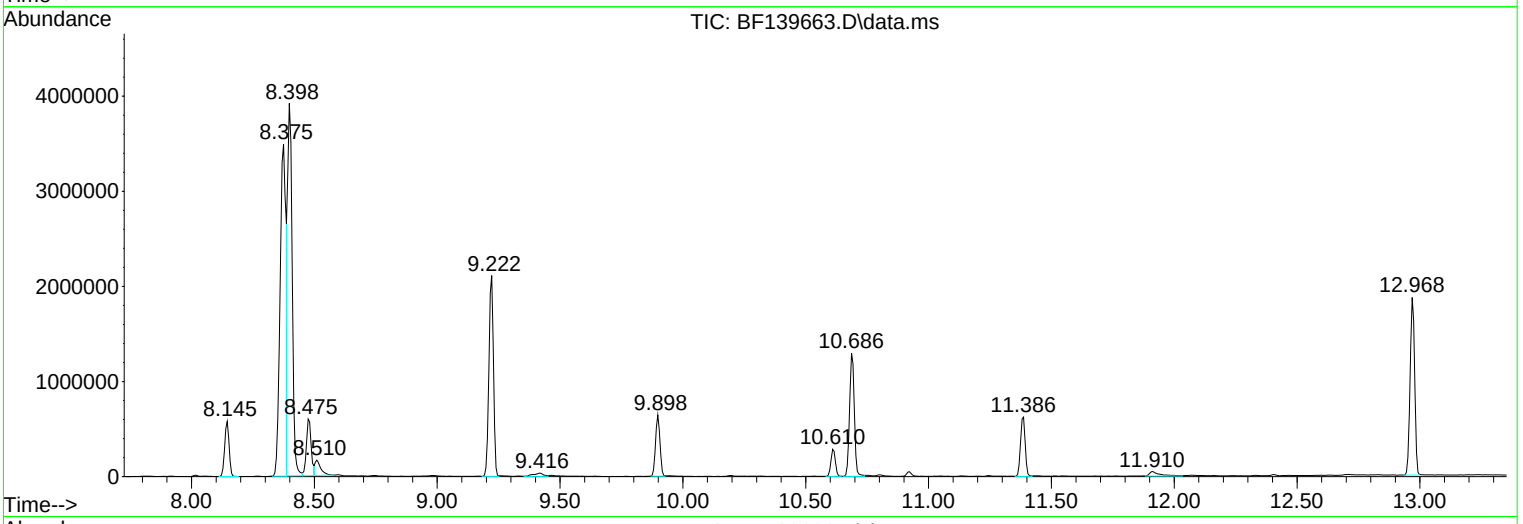
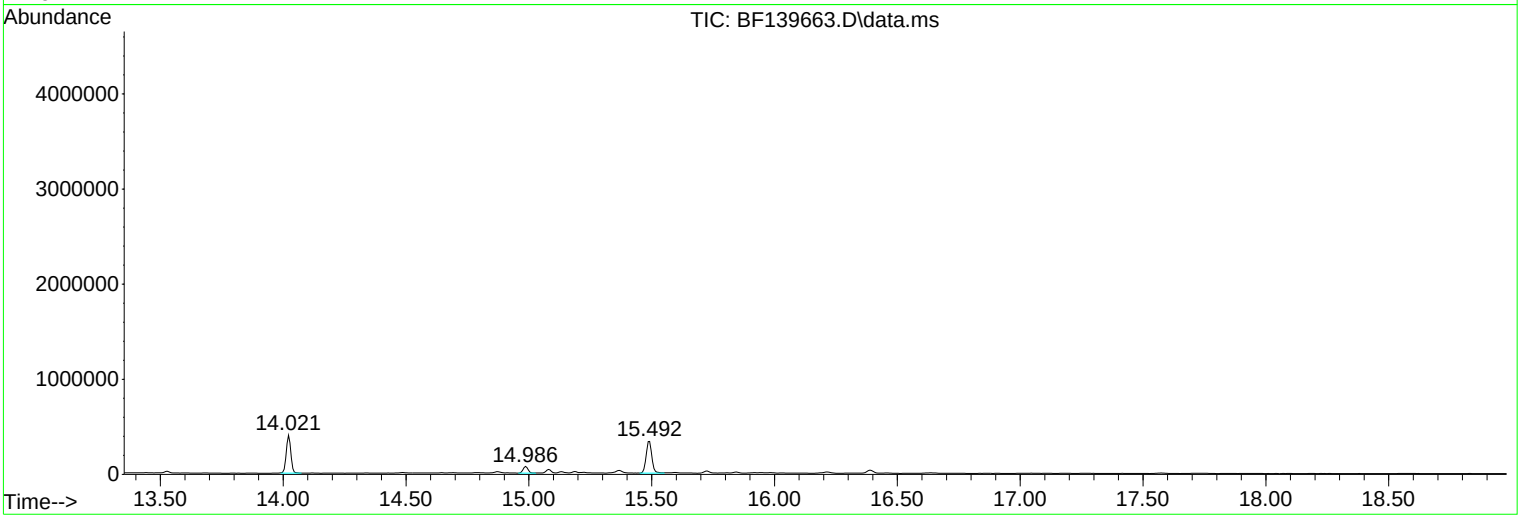
ClientSampleId :
MH-147

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.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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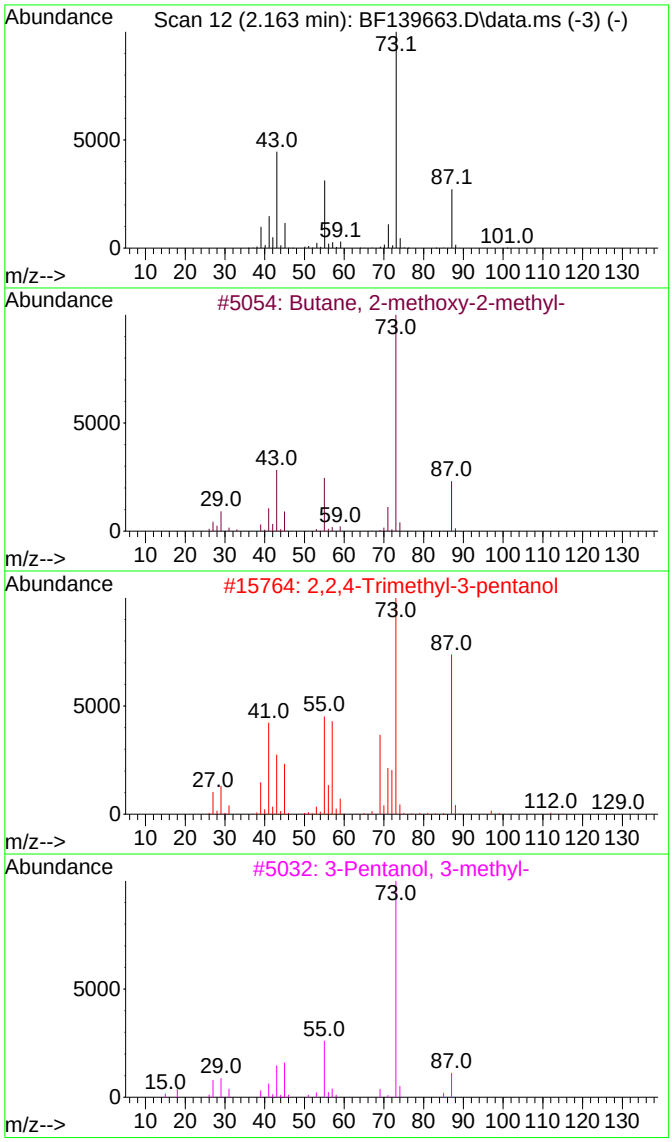
TIC Integration Parameters: LSCINT.P

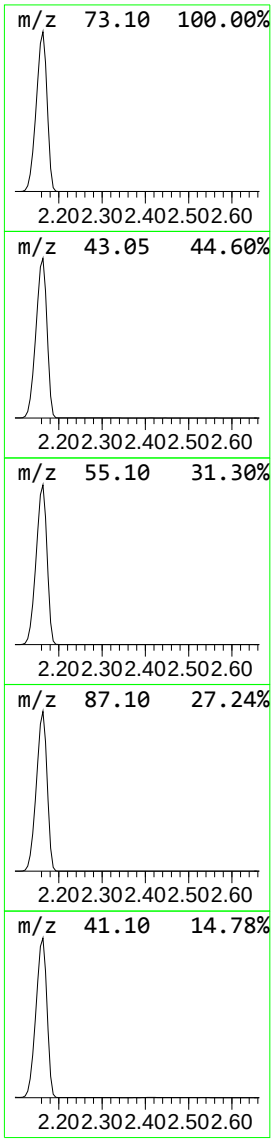
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	289.33 ng	8070730	1,4-Dichlorobenzene-d4	6.863

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	39
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Operator : RC/JU
Sample : P4254-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-147

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.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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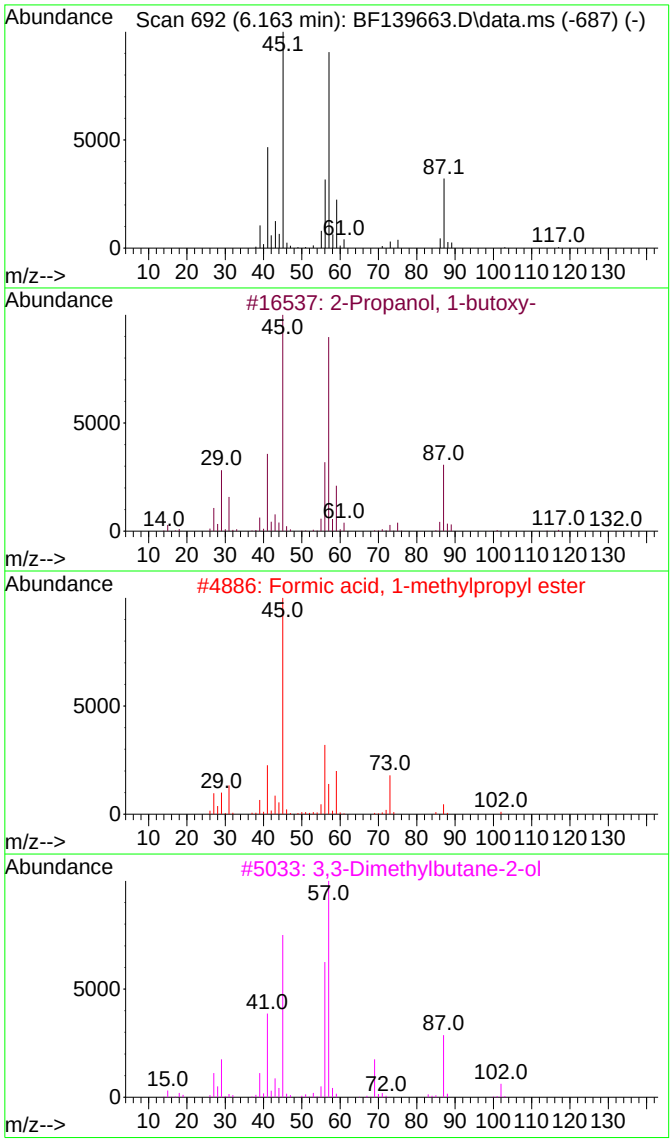
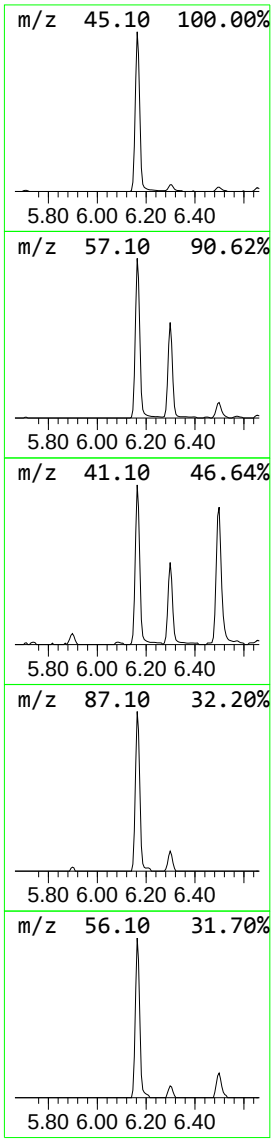
Peak Number 2 2-Propanol, 1-butoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.163	6.90 ng	192392	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	90
2	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	59
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
4	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	53
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	42





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Acq On : 04 Oct 2024 17:55
Operator : RC/JU
Sample : P4254-05
Misc :
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Instrument :
BNA_F
ClientSampleId :
MH-147

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.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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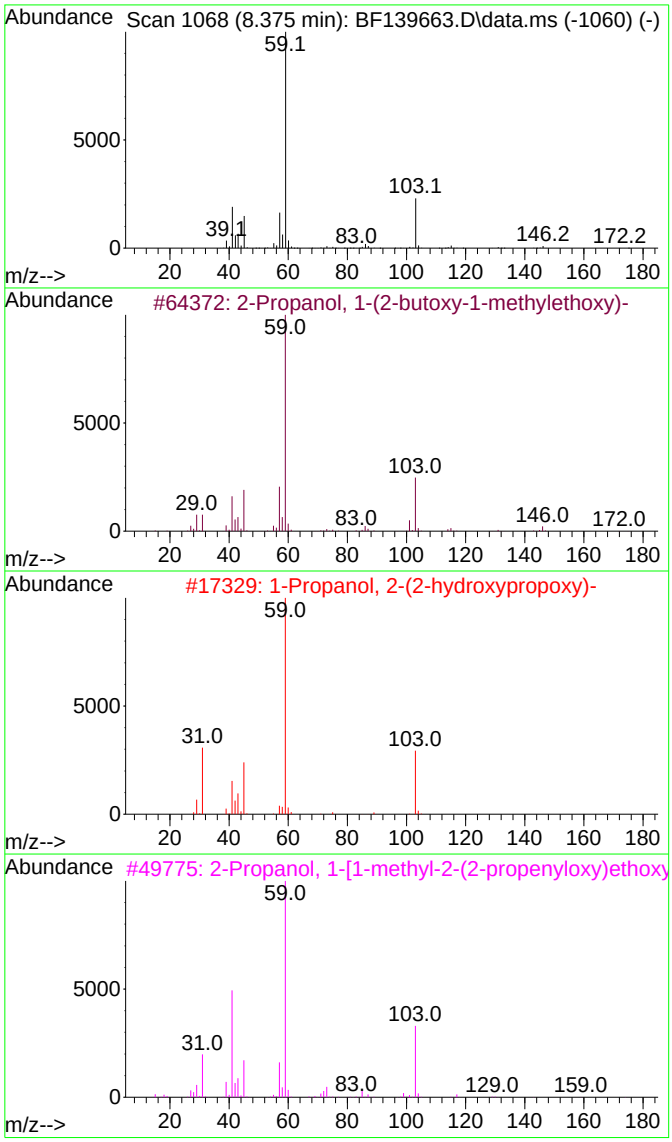
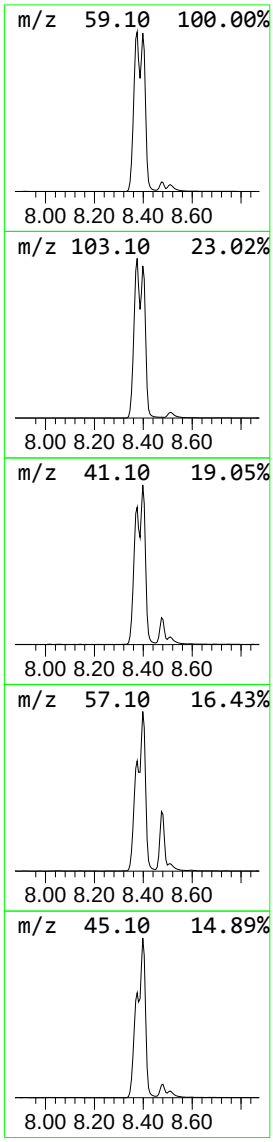
Peak Number 3 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.375	165.55 ng	5990730	Naphthalene-d8	8.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	83
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	74
4	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1010367-13-4	64
5	Propane, 1,2-dimethoxy-	104	C5H12O2	007778-85-0	64





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Sample : P4254-05
Misc :
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Instrument :
BNA_F
ClientSampleId :
MH-147

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.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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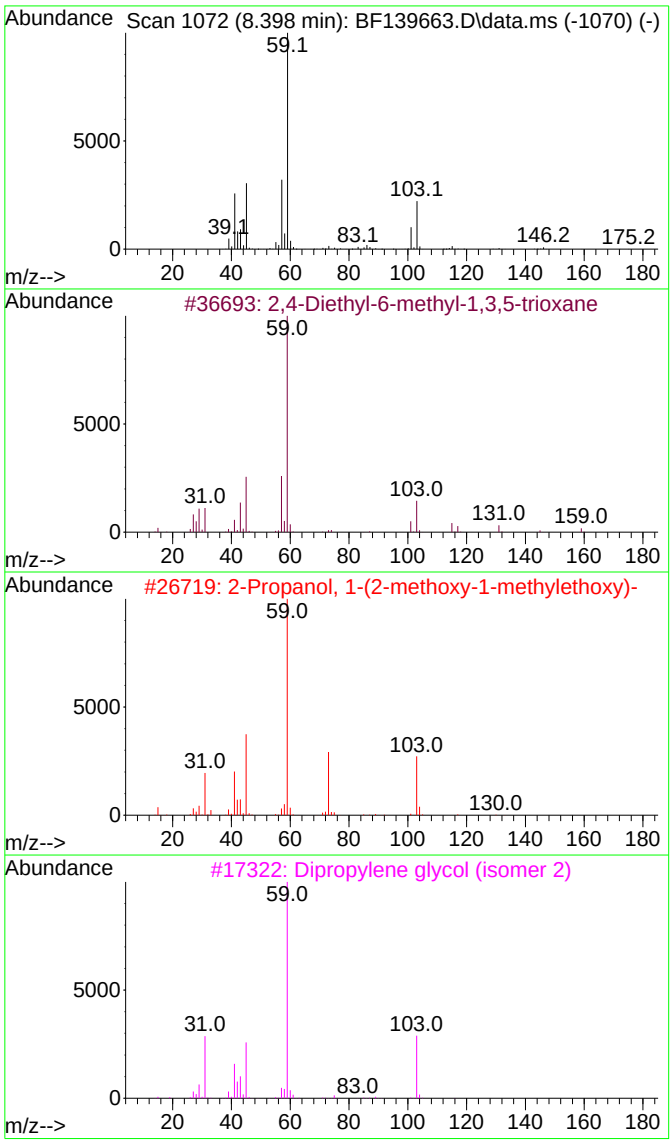
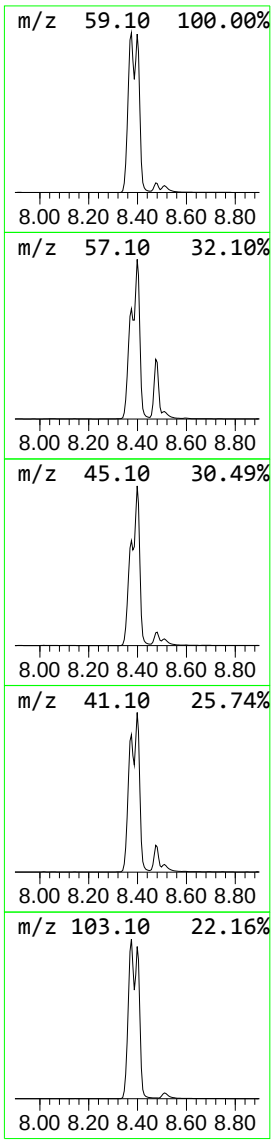
Peak Number 4 2,4-Diethyl-6-methyl-1,3,5-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.398	136.14 ng	4926520	Naphthalene-d8	8.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Diethyl-6-methyl-1,3,5-trioxane	160	C8H16O3	117888-04-7	78
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
3	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64





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Sample : P4254-05
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.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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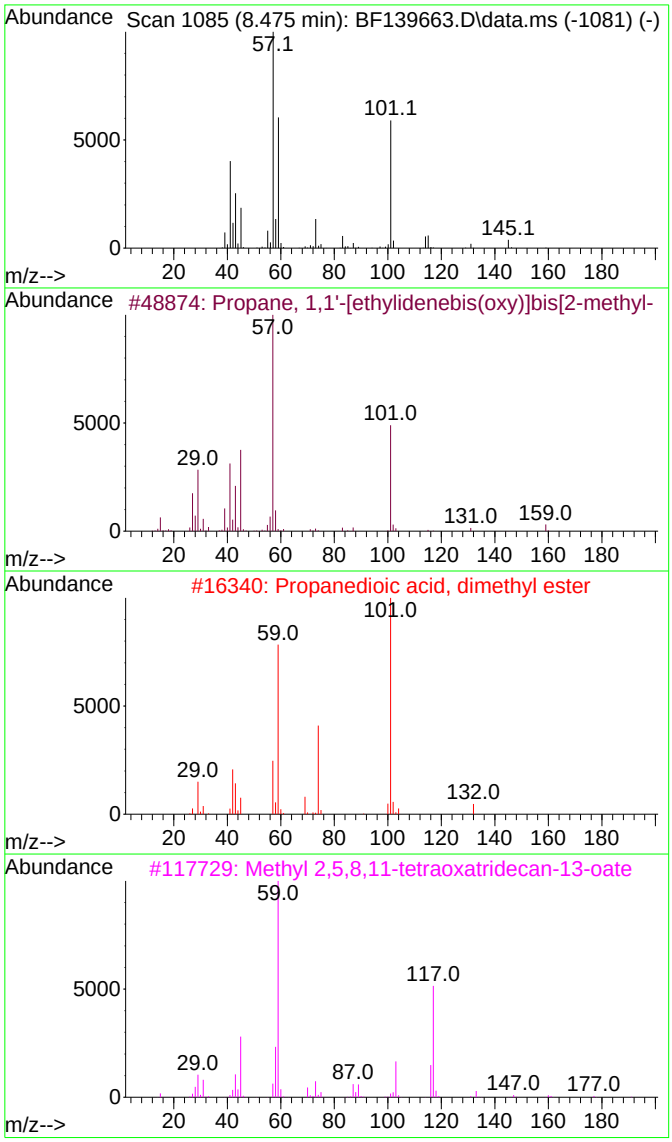
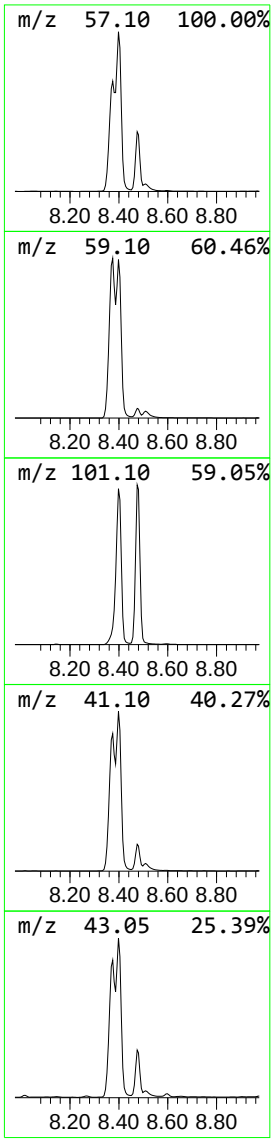
Peak Number 5 unknown8.475 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.475	22.33 ng	807963	Naphthalene-d8	8.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1'-[ethylidenebis(oxy...	174	C10H22O2	005669-09-0	37
2	Propanedioic acid, dimethyl ester	132	C5H8O4	000108-59-8	36
3	Methyl 2,5,8,11-tetraoxatridecan...	236	C10H20O6	1000366-78-2	35
4	Hydrazine, 1,1-dimethyl-2-propyl-	102	C5H14N2	052728-54-8	35
5	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	35





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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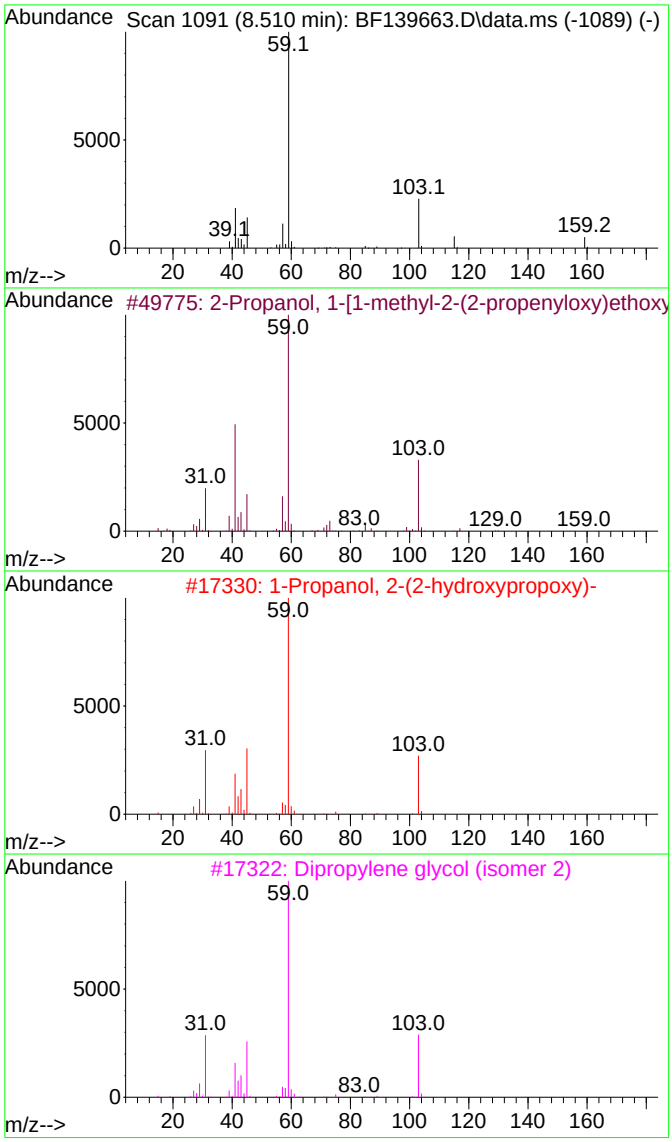
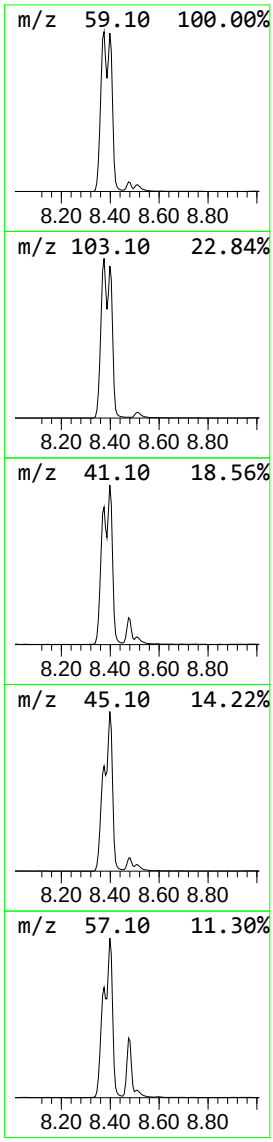
Peak Number 6 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.510	7.14 ng	258253	Naphthalene-d8	8.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	78
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
3	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	72
4	Methane, diethoxy-	104	C5H12O2	000462-95-3	64
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	56





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Sample : P4254-05
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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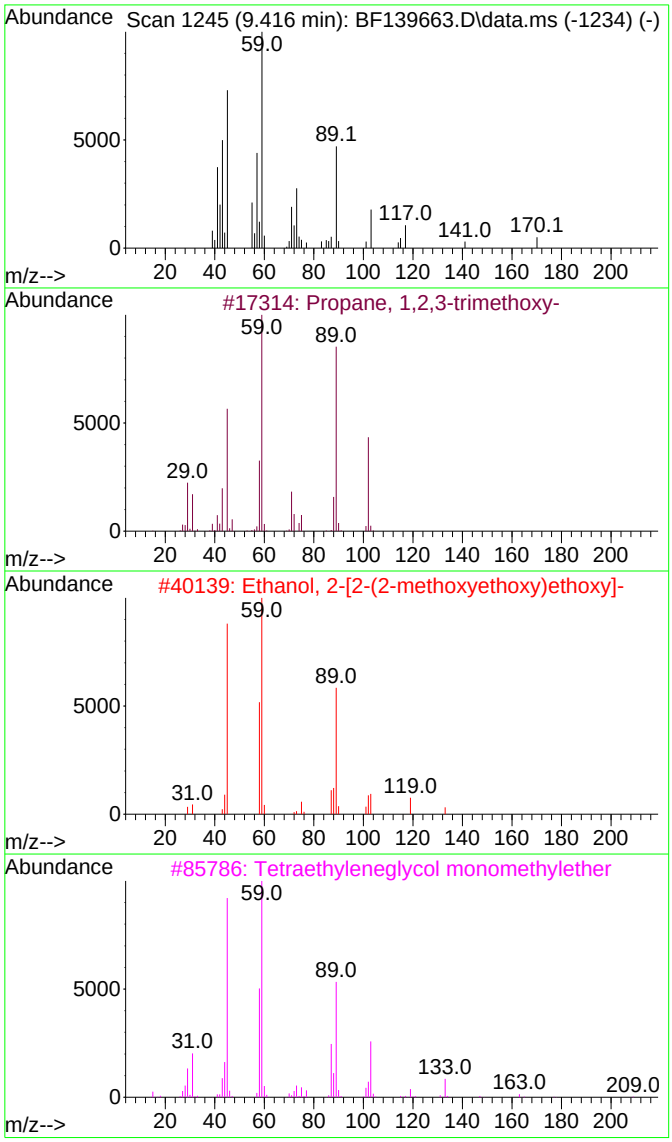
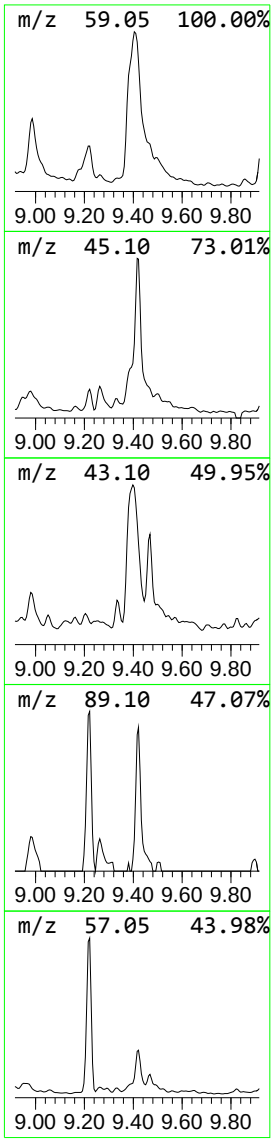
Peak Number 7 unknown9.416 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.416	2.35 ng	92836	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,2,3-trimethoxy-	134	C6H14O3	020637-49-4	45
2	Ethanol, 2-[2-(2-methoxyethoxy)e...	164	C7H16O4	000112-35-6	40
3	Tetraethyleneglycol monomethylether	208	C9H20O5	023783-42-8	40
4	2-Ethyl-4,6-dimethyl-1,3,5-trioxane	146	C7H14O3	024261-86-7	40
5	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	38





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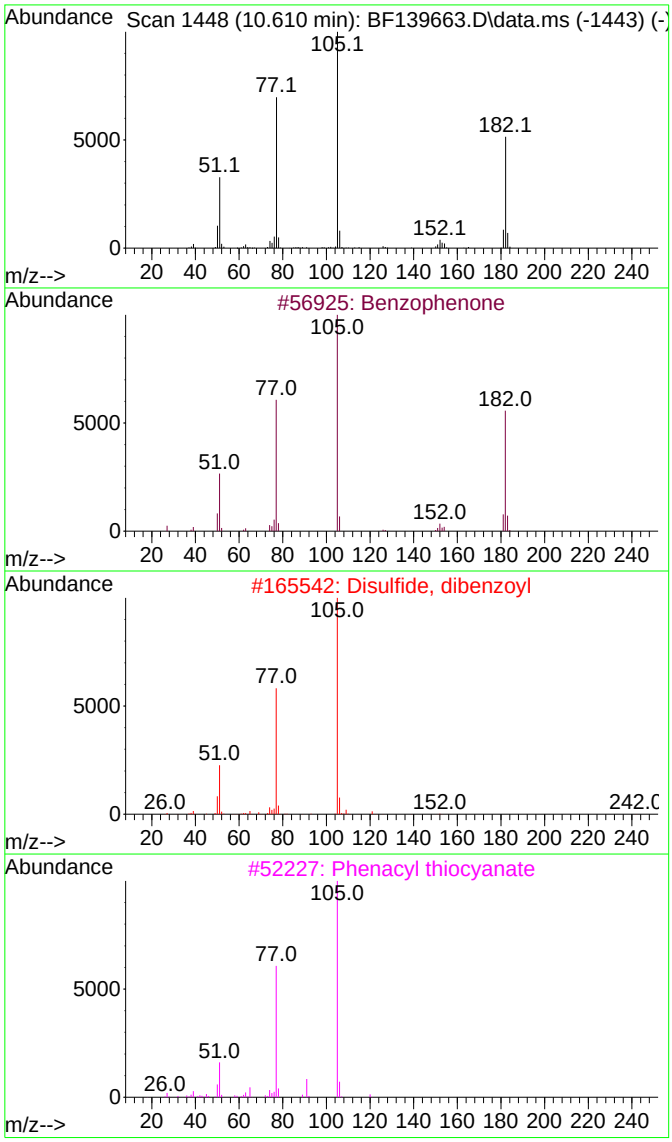
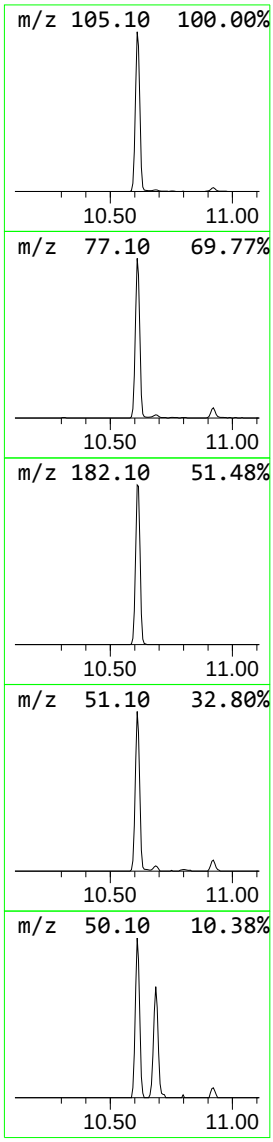
Peak Number 8 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	9.05 ng	358196	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	52
3	Phenacyl thiocyanate	177	C9H7NOS	005399-30-4	50
4	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	50
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
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MH-147

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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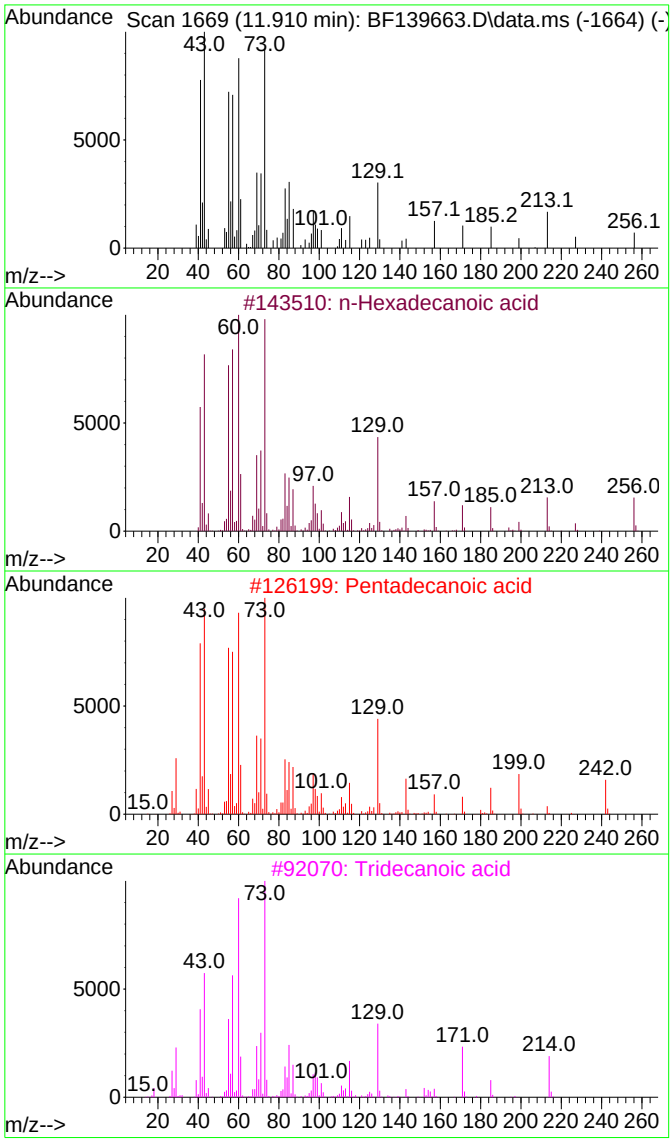
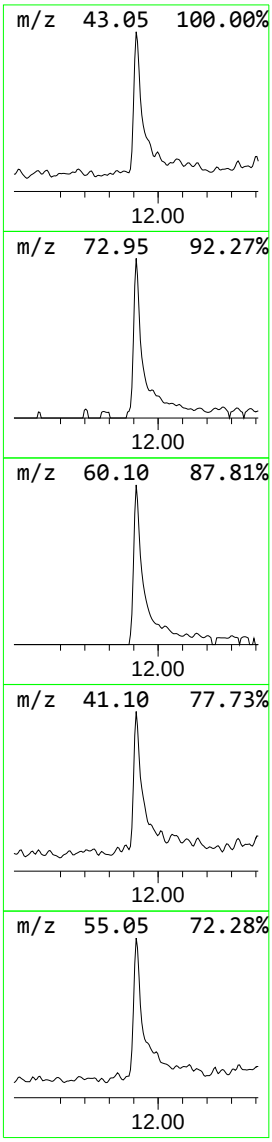
Peak Number 9 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	3.28 ng	132092	Phenanthrene-d10	11.386

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	74
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	50





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Data File : BF139663.D
Acq On : 04 Oct 2024 17:55
Operator : RC/JU
Sample : P4254-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-147

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

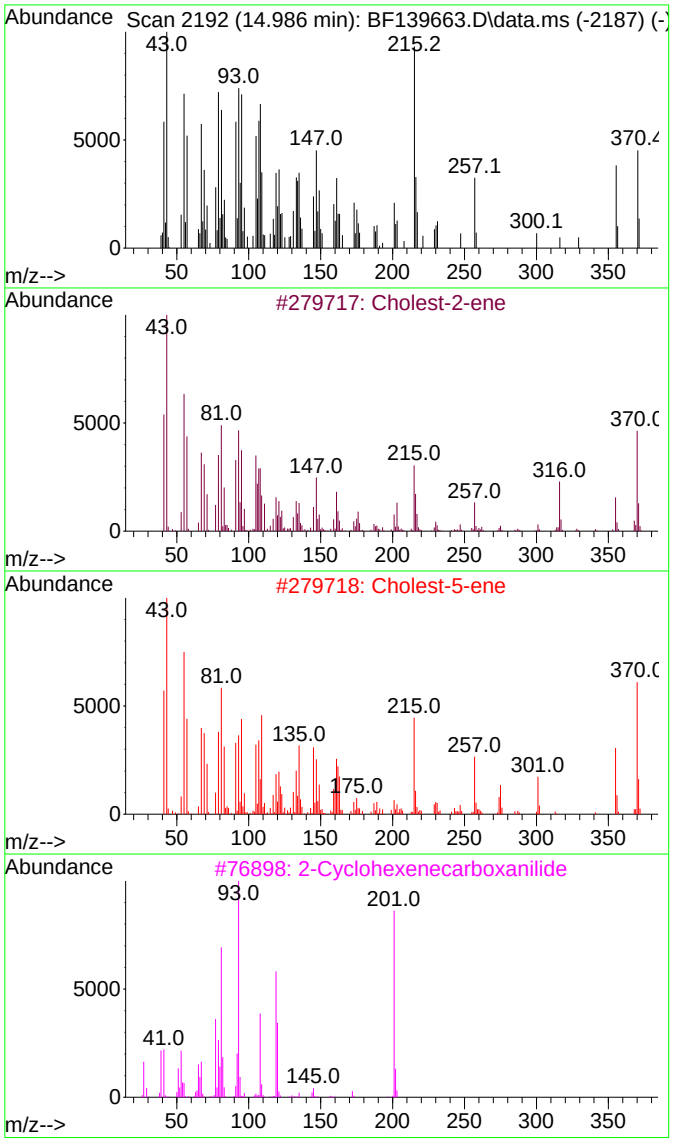
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

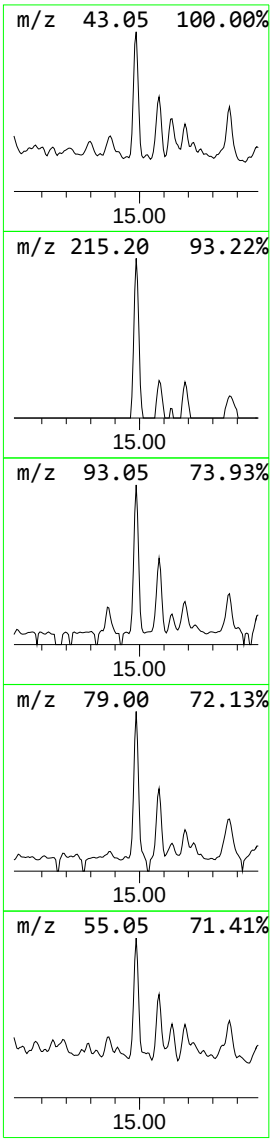
****

Peak Number 10 Cholest-2-ene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.986	3.58 ng	96667	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-2-ene	370	C27H46	015910-23-3	90
2	Cholest-5-ene	370	C27H46	000570-74-1	62
3	2-Cyclohexenecarboxanilide	201	C13H15NO	1000160-08-2	56
4	Cholan-24-oic acid, 3,12-bis(ace...	490	C29H46O6	001181-44-8	53
5	Allopregnan-3.alpha.-ol-20-one	318	C21H34O2	000516-54-1	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100424\
Data File : BF139663.D
Acq On : 04 Oct 2024 17:55
Operator : RC/JU
Sample : P4254-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-147

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.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	289.3	ng	8070730	1	6.863	557890	20.0
2-Propanol, 1-b...	6.163	6.9	ng	192392	1	6.863	557890	20.0
2-Propanol, 1-(...	8.375	165.6	ng	5990730	2	8.145	723754	20.0
2,4-Diethyl-6-m...	8.398	136.1	ng	4926520	2	8.145	723754	20.0
unknown8.475	8.475	22.3	ng	807963	2	8.145	723754	20.0
2-Propanol, 1-[...	8.510	7.1	ng	258253	2	8.145	723754	20.0
unknown9.416	9.416	2.4	ng	92836	3	9.898	791500	20.0
Benzophenone	10.610	9.1	ng	358196	3	9.898	791500	20.0
n-Hexadecanoic ...	11.910	3.3	ng	132092	4	11.386	806118	20.0
Cholest-2-ene	14.986	3.6	ng	96667	6	15.492	539744	20.0