LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
Data File : BF126649.D
Acq On : 24 Jan 2022 19:51
Operator : CG/JU
Sample : N1217-08
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-242

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-BF011822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126649.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	22	rVB	141913	246736	1.47%	0.597%
2	5.581	586	594	605	rBV2	486833	1160769	6.93%	2.810%
3	5.951	645	657	660	rBV	4313765	9035714	53.96%	21.875%
4	6.245	703	707	713	rVB	830472	817198	4.88%	1.978%
5	6.569	759	762	768	rVB	1332765	1118014	6.68%	2.707%
6	6.963	825	829	833	rBV	836478	670059	4.00%	1.622%
7	7.075	845	848	850	rBV	268660	241027	1.44%	0.584%
8	7.363	890	897	899	rBV	237683	266487	1.59%	0.645%
9	7.492	914	919	921	rBV2	213034	250813	1.50%	0.607%
10	7.522	921	924	926	rVV	874759	715453	4.27%	1.732%
11	7.551	926	929	933	rVB	260778	257348	1.54%	0.623%
12	7.886	983	986	990	rBV3	209982	268281	1.60%	0.650%
13	8.145	1027	1030	1036	rBV	1456887	1522423	9.09%	3.686%
14	8.222	1040	1043	1045	rVV2	433312	496681	2.97%	1.202%
15	8.245	1045	1047	1050	rVV	1035875	955343	5.70%	2.313%
16	8.298	1053	1056	1059	rVB3	408377	395378	2.36%	0.957%
17	8.486	1084	1088	1090	rBV3	286745	347168	2.07%	0.840%
18	8.539	1092	1097	1100	rVV5	256639	576852	3.44%	1.397%
19	14.821	2157	2165	2168	rVB	9580799	16746176	100.00%	40.543%
20	14.945	2183	2186	2190	rVV2	1399104	1496330	8.94%	3.623%
21	14.992	2190	2194	2199	rVB	3368984	3720933	22.22%	9.008%

Sum of corrected areas: 41305183

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012422\
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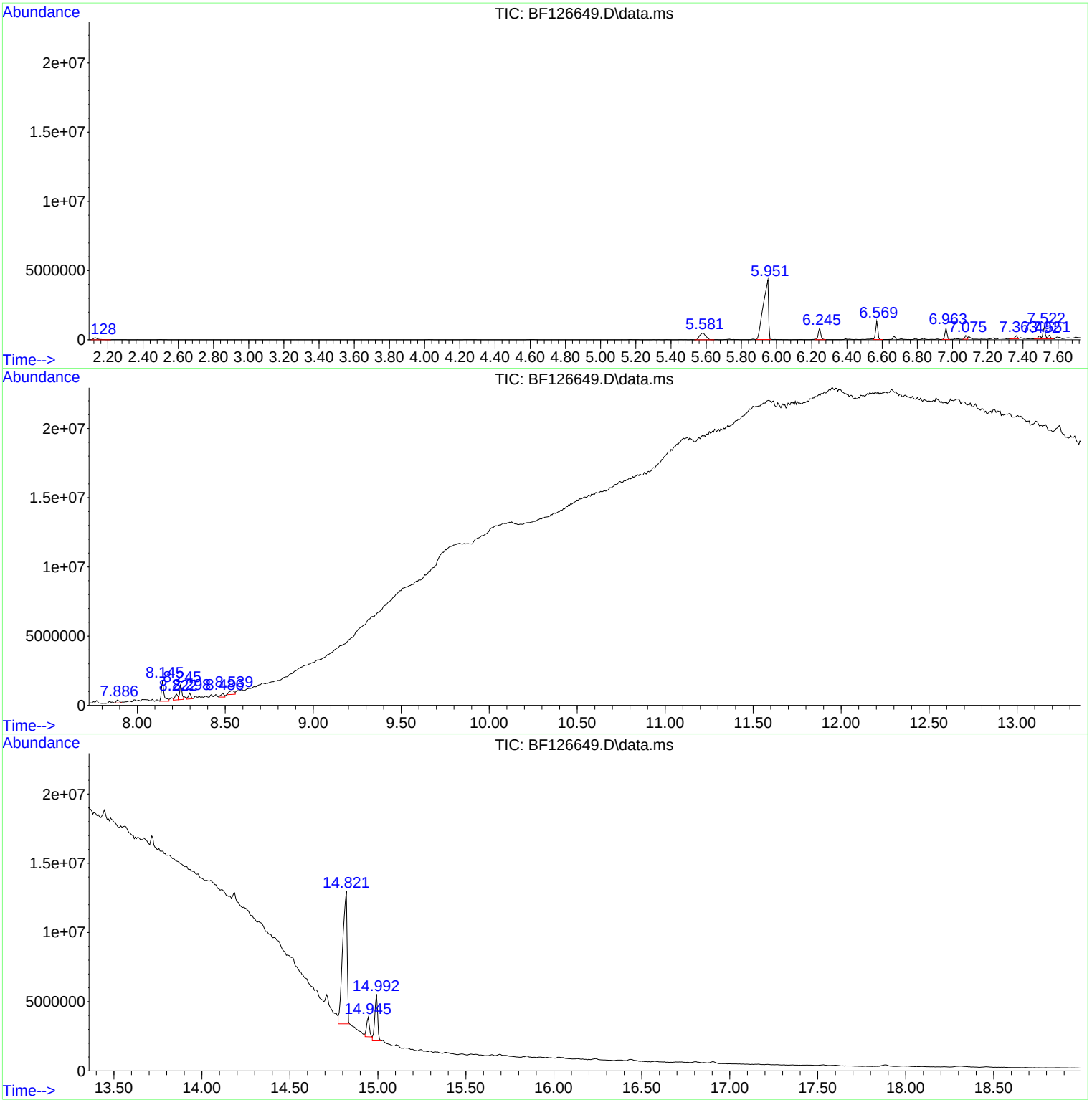
BNA_F
ClientSampleId :
VNJ-242

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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 : BF126649.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

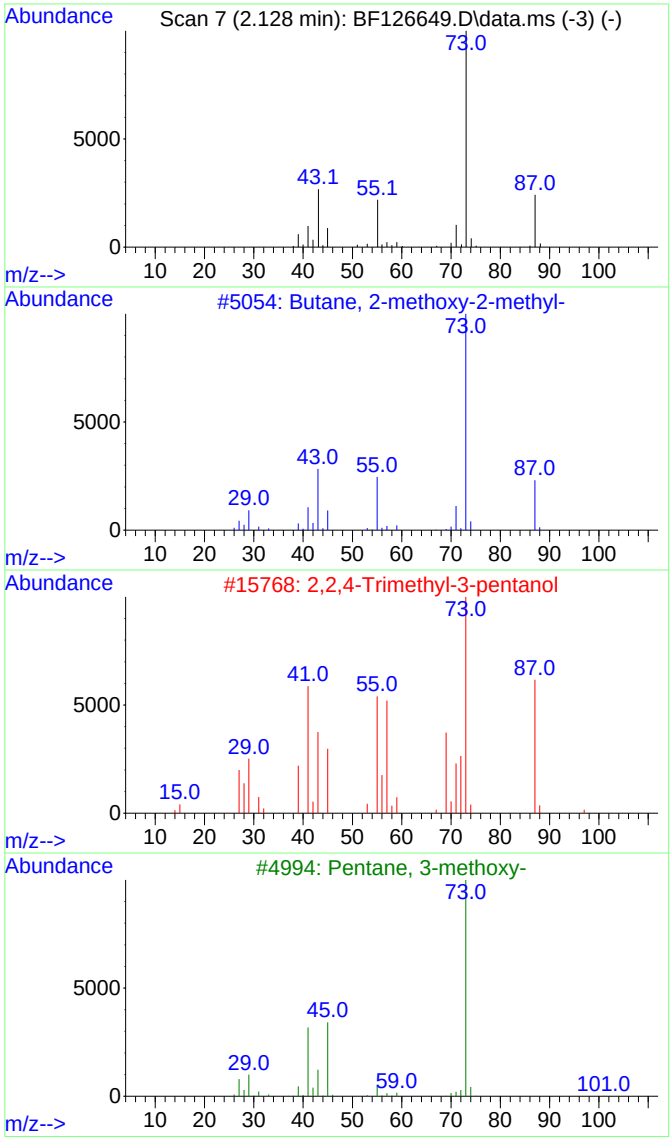
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

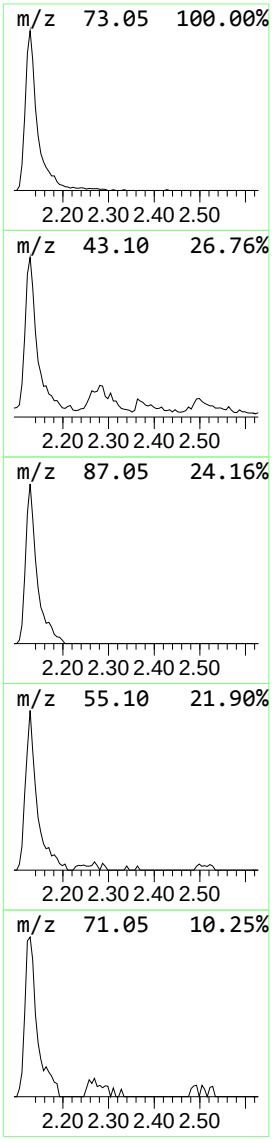
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	7.36 ng	246736	1,4-Dichlorobenzene-d4	6.963

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	56
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10





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VNJ-242

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

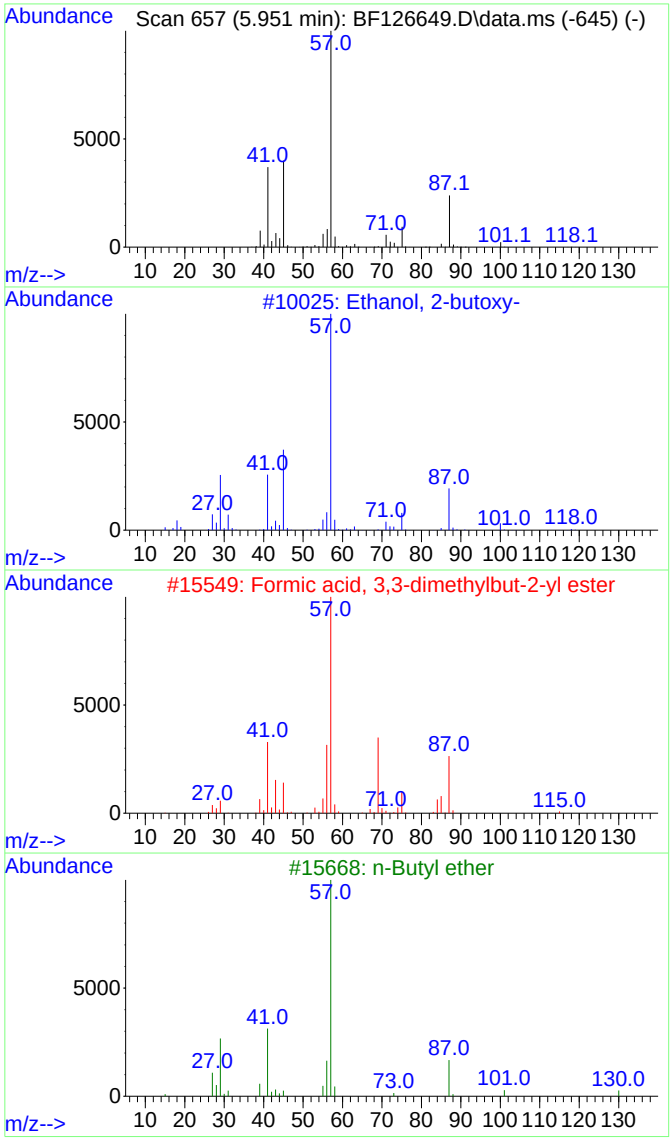
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

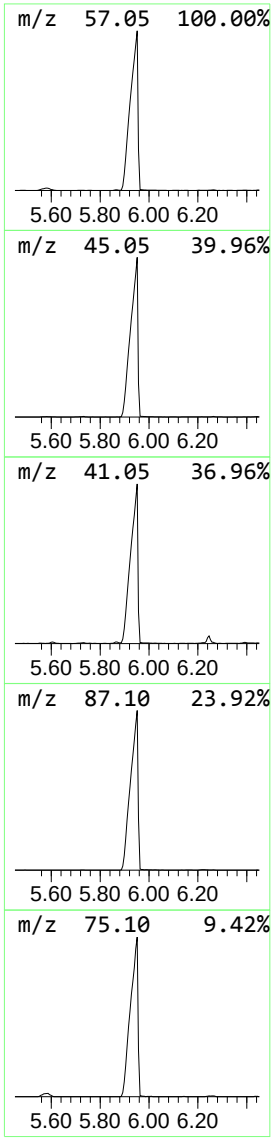
****

Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.951	269.70 ng	9035710	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2	Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	72
3	n-Butyl ether	130	C8H18O	000142-96-1	25
4	Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	17
5	1,3-Propanediol, 2-methyl-, dipr...	202	C10H18O4	054932-83-1	12





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Operator : CG/JU
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Instrument :
BNA_F
ClientSampleId :
VNJ-242

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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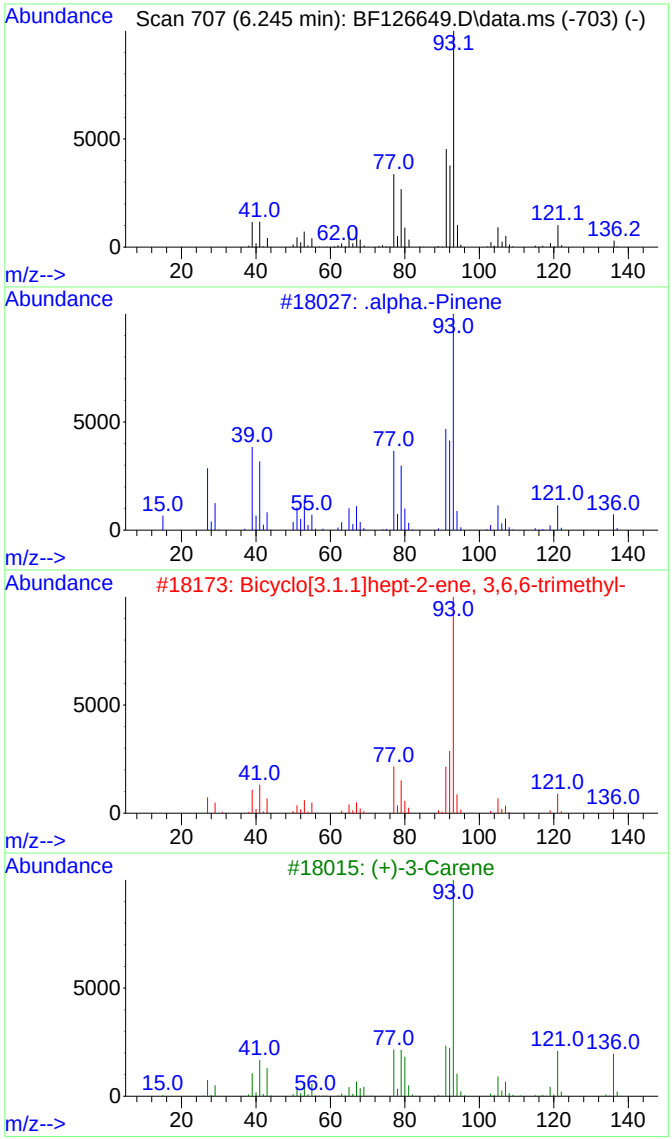
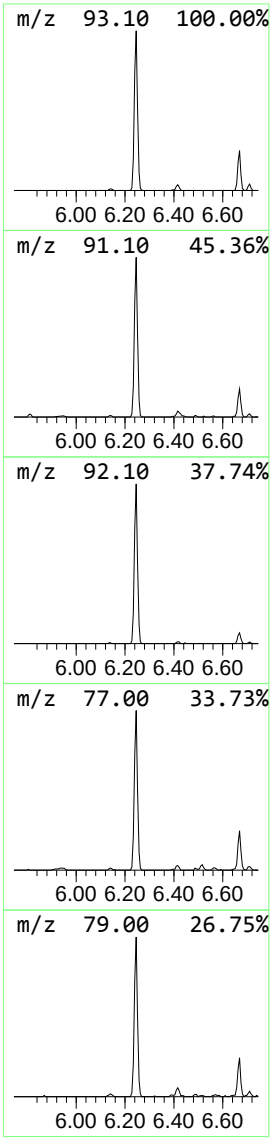
****

Peak Number 3 .alpha.-Pinene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.245	24.39 ng	817198	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	94
2	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
3	(+)-3-Carene	136	C10H16	000498-15-7	87
4	Cyclohexene, 4-methylene-1-(1-me...	136	C10H16	000099-84-3	87
5	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	86





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

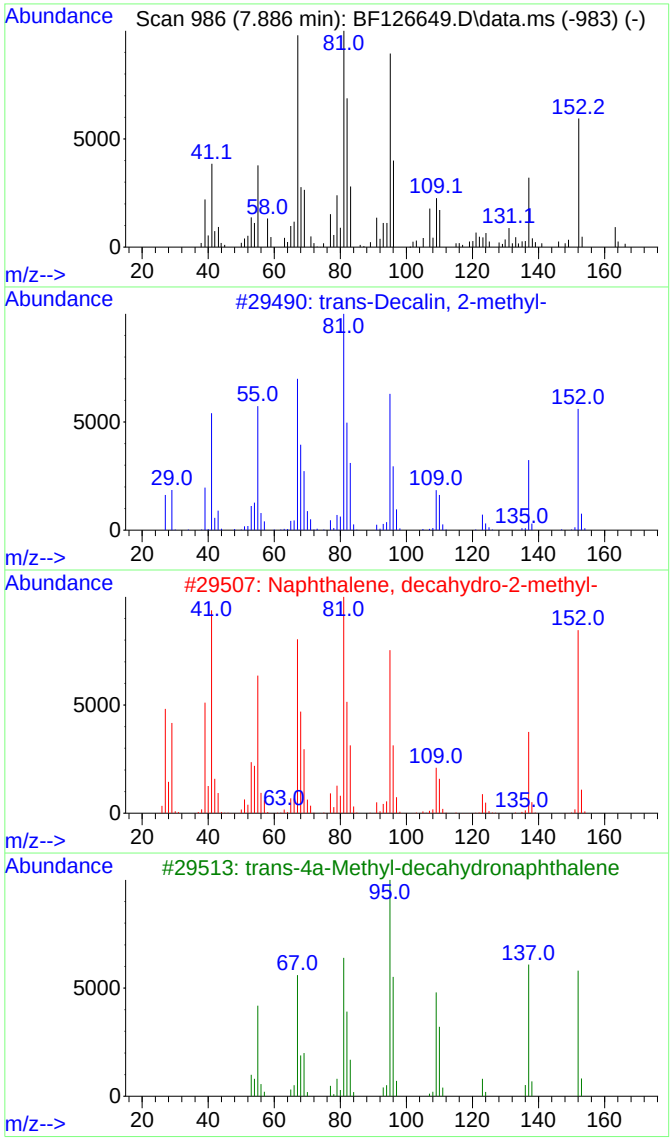
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

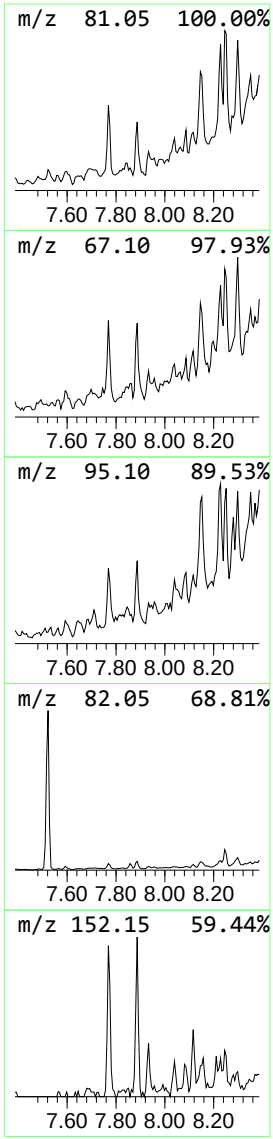
****

Peak Number 4 trans-Decalin, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.886	5.62 ng	268281	Naphthalene-d8	8.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	91
2	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	83
3	trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	76
4	Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	68
5	Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-25-0	62





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

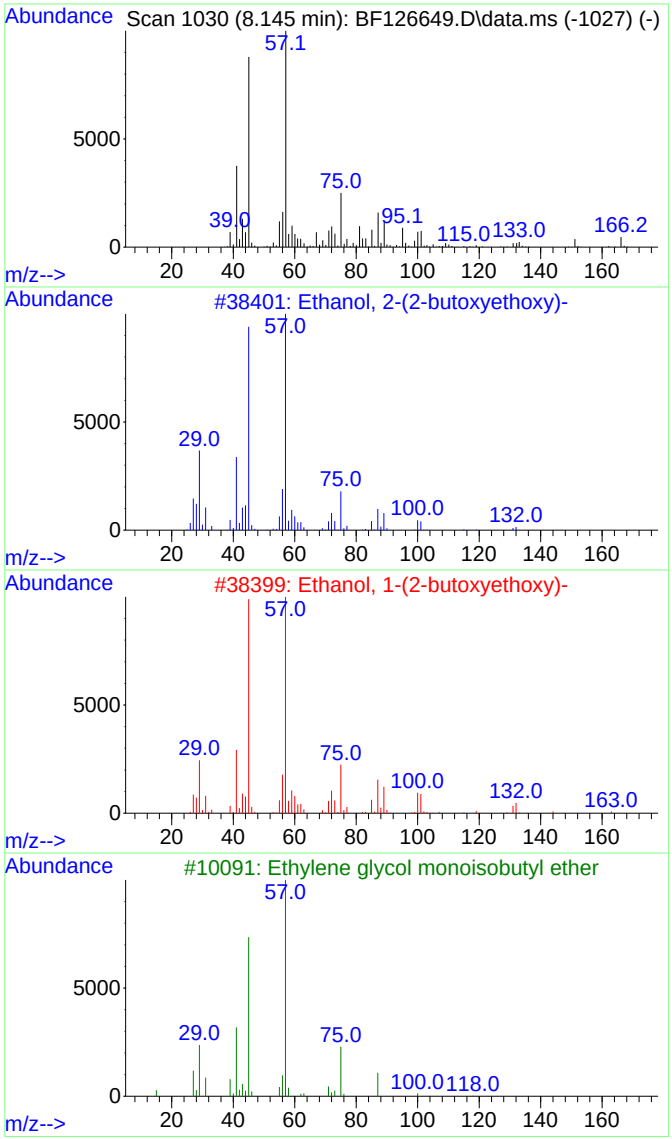
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

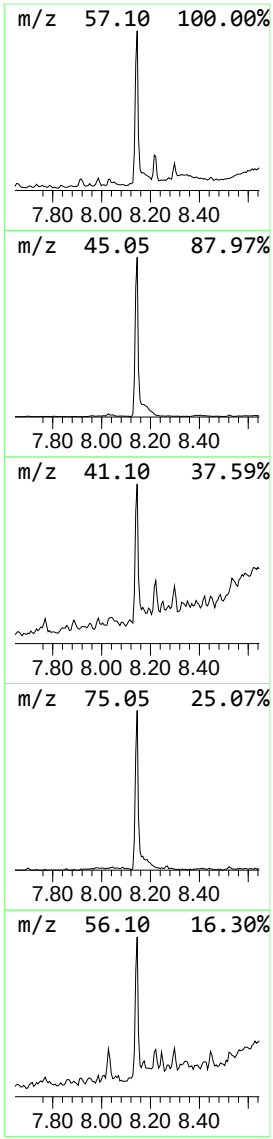
****

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.145	31.87 ng	1522420	Naphthalene-d8	8.245

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	90
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	47
5	Tetraethylene glycol	194	C8H18O5	000112-60-7	47





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Instrument :
BNA_F
ClientSampleId :
VNJ-242

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

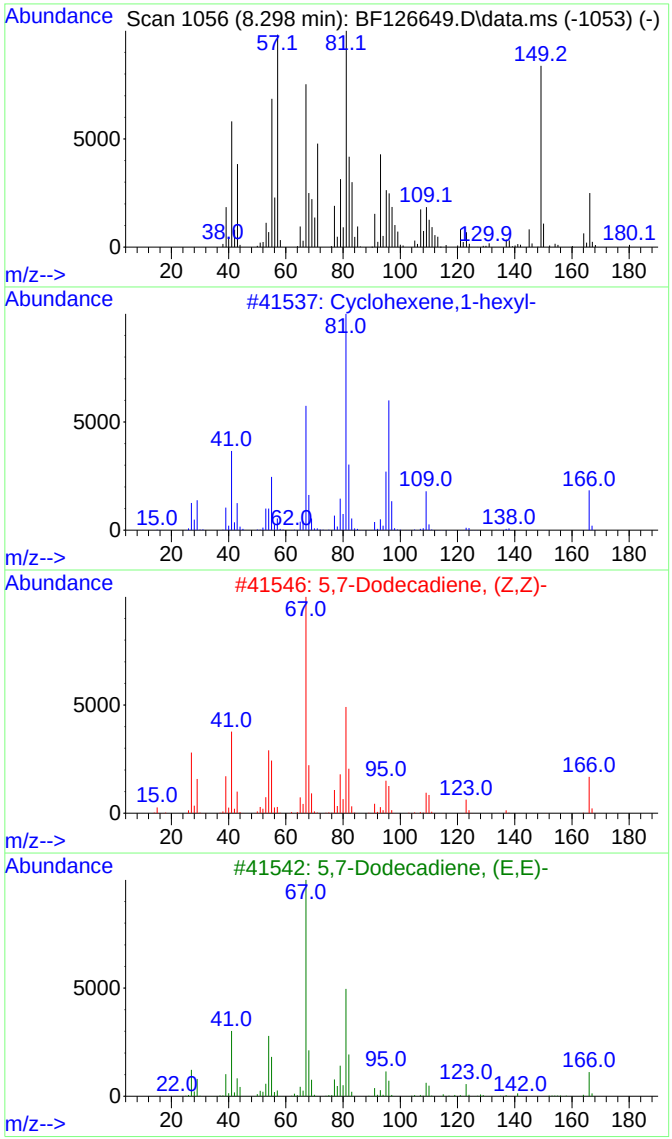
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

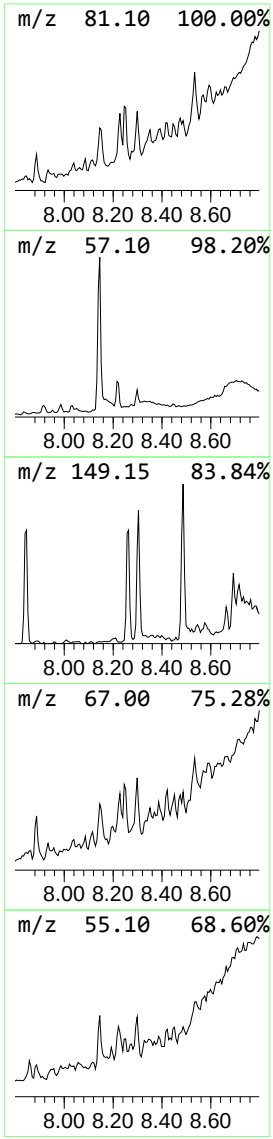
****

Peak Number 6 Cyclohexene,1-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.298	8.28 ng	395378	Naphthalene-d8	8.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene,1-hexyl-	166	C12H22	003964-66-7	55
2	5,7-Dodecadiene, (Z,Z)-	166	C12H22	006108-62-9	42
3	5,7-Dodecadiene, (E,E)-	166	C12H22	030651-68-4	30
4	Spiro[5.6]dodecane	166	C12H22	000181-15-7	27
5	Cycloundecene, 1-methyl-	166	C12H22	088828-82-4	25





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ClientSampleId :
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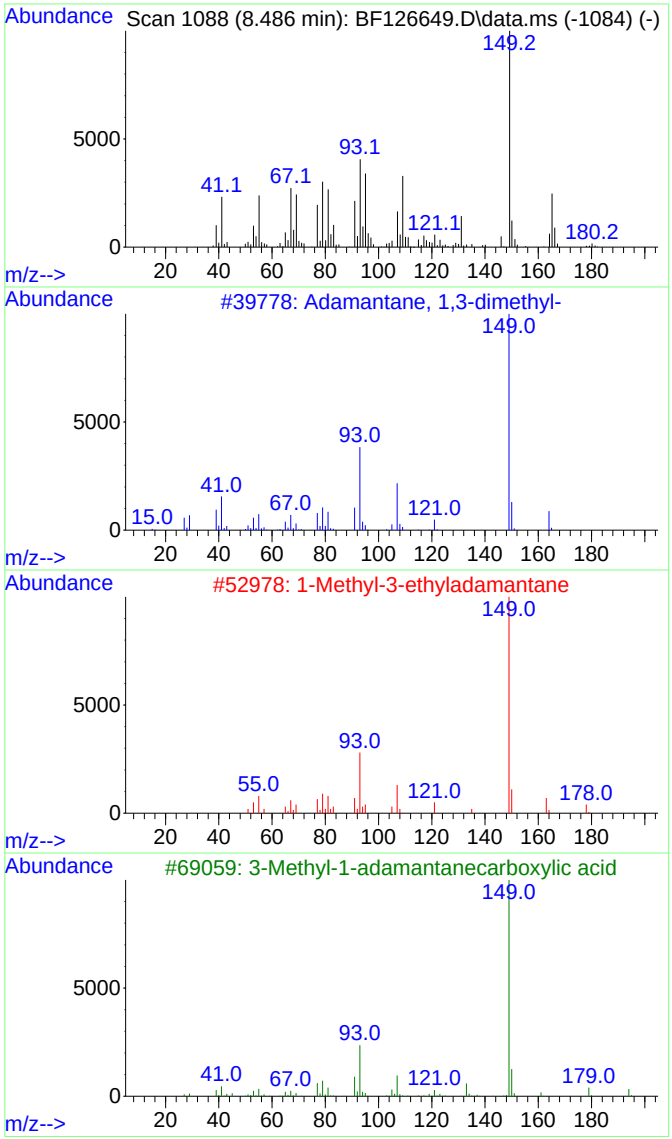
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

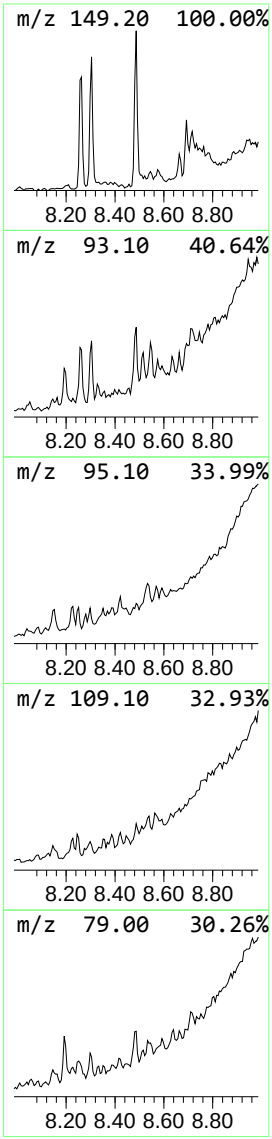
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Adamantane, 1,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.486	7.27 ng	347168	Naphthalene-d8	8.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	52
2	1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	50
3	3-Methyl-1-adamantanecarboxylic ...	194	C12H18O2	1000504-38-9	50
4	Added stereo to name	164	C12H20	024145-88-8	49
5	1H-Purin-6-amine, N-methyl-	149	C6H7N5	000443-72-1	43





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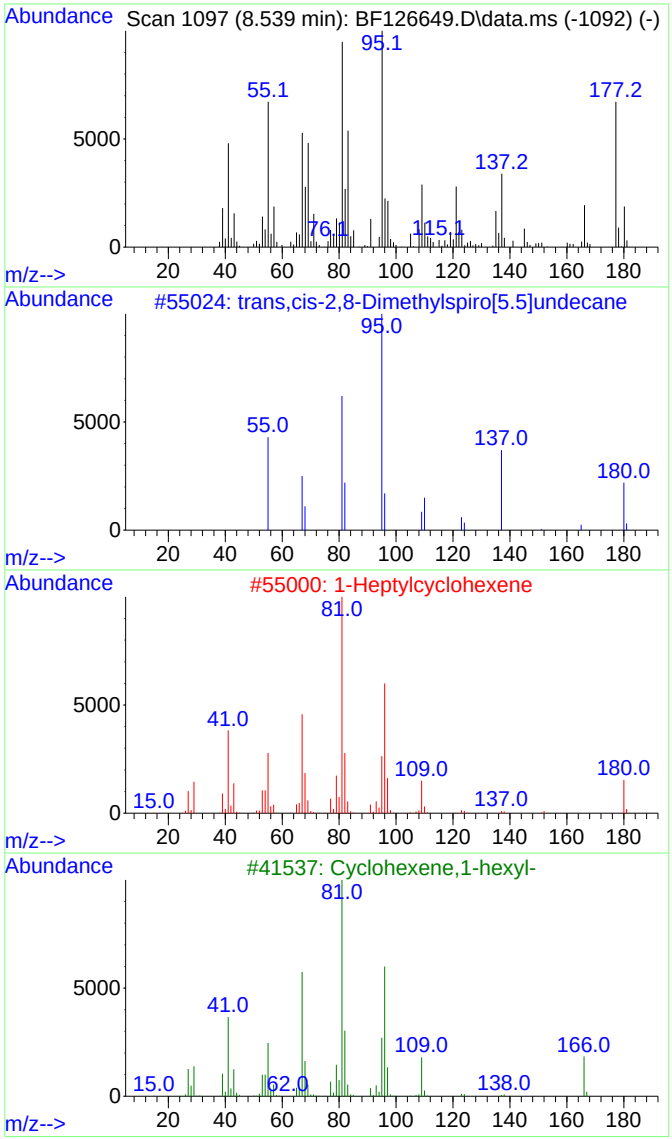
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

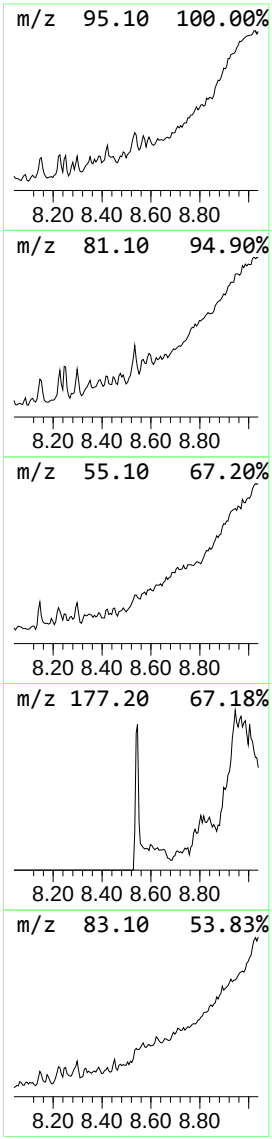
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 trans,cis-2,8-Dimethylspiro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.539	12.08 ng	576852	Naphthalene-d8	8.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans,cis-2,8-Dimethylspiro[5.5]...	180	C13H24	095472-52-9	55
2	1-Heptylcyclohexene	180	C13H24	015232-86-7	41
3	Cyclohexene,1-hexyl-	166	C12H22	003964-66-7	41
4	Naphthalene, decahydro-1,6-dimet...	166	C12H22	001750-51-2	38
5	cis,cis-2,8-Dimethylspiro[5.5]un...	180	C13H24	095530-75-9	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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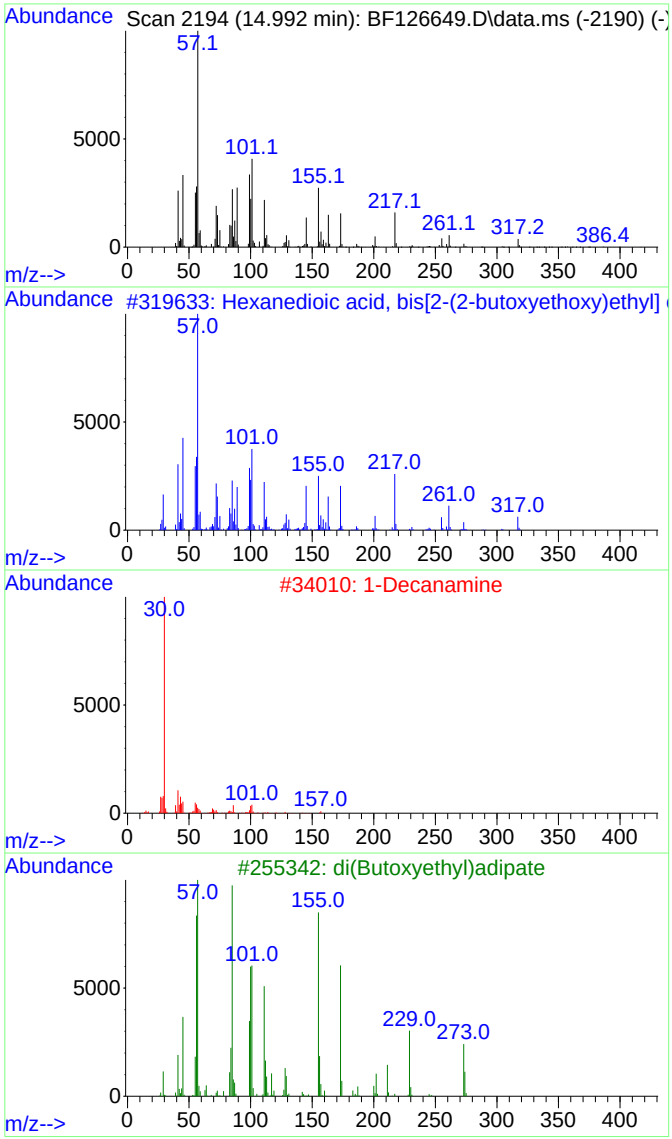
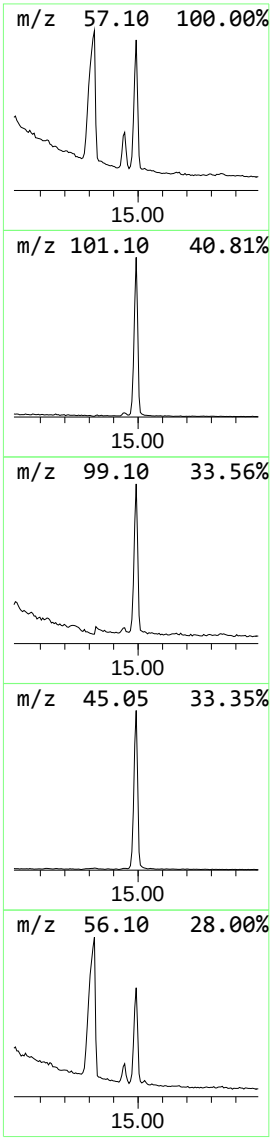
Peak Number 9 unknown14.992 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.992	20.00 ng	3720930	Perylene-d12	15.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis[2-(2-butox...	434	C22H42O8	000141-17-3	35
2	1-Decanamine	157	C10H23N	002016-57-1	22
3	di(Butoxyethyl)adipate	346	C18H34O6	000141-18-4	17
4	Succinic acid, 2,2-dichloroethyl...	326	C14H24Cl2O4	1000389-54-2	12
5	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	12





Tentatively Identified Compound (LSC) summary

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Data File : BF126649.D
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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...	2.128	7.4	ng	246736	1	6.963	670059	20.0
Ethanol, 2-butoxy-	5.951	269.7	ng	9035710	1	6.963	670059	20.0
.alpha.-Pinene	6.245	24.4	ng	817198	1	6.963	670059	20.0
trans-Decalin, ...	7.886	5.6	ng	268281	2	8.245	955343	20.0
Ethanol, 2-(2-b...	8.145	31.9	ng	1522420	2	8.245	955343	20.0
Cyclohexene,1-h...	8.298	8.3	ng	395378	2	8.245	955343	20.0
Adamantane, 1,3...	8.486	7.3	ng	347168	2	8.245	955343	20.0
trans,cis-2,8-D...	8.539	12.1	ng	576852	2	8.245	955343	20.0
unknown14.992	14.992	20.0	ng	3720930	6	15.692	3720930	20.0