LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099162.D
Acq On : 6 Oct 2017 22:07
Operator : SJ/JU
Sample : I5516-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	2.169	8	14	23	rVB	674054	841622	22.47%	2.774%
2	5.087	506	510	519	rBV	322877	359018	9.59%	1.183%
3	5.487	573	578	581	rBV	1778470	1782465	47.59%	5.875%
4	6.487	744	748	761	rVB	1310878	1203540	32.13%	3.967%
5	6.634	768	773	776	rBV	3057556	2915913	77.85%	9.612%
6	6.687	780	782	787	rVB2	33636	37735	1.01%	0.124%
7	6.787	794	799	802	rBV	34722	38453	1.03%	0.127%
8	6.863	808	812	815	rBV	889021	726839	19.41%	2.396%
9	7.022	834	839	842	rVB	2857720	2655373	70.90%	8.753%
10	7.428	901	908	911	rVB	2079426	2222694	59.35%	7.327%
11	7.510	918	922	926	rBV3	31954	52290	1.40%	0.172%
12	7.551	926	929	933	rVB2	33891	43727	1.17%	0.144%
13	7.722	953	958	965	rBV3	38581	63938	1.71%	0.211%
14	7.798	965	971	975	rVV6	19121	40854	1.09%	0.135%
15	7.875	978	984	992	rBV4	45564	89589	2.39%	0.295%
16	8.045	1008	1013	1016	rBV2	78048	108241	2.89%	0.357%
17	8.075	1016	1018	1022	rVB3	46625	51400	1.37%	0.169%
18	8.145	1025	1030	1033	rBV	1165107	1047717	27.97%	3.454%
19	8.269	1047	1051	1054	rBV2	30962	39346	1.05%	0.130%
20	8.322	1058	1060	1068	rVV7	42107	91805	2.45%	0.303%
21	8.386	1068	1071	1074	rVB2	47789	43306	1.16%	0.143%
22	8.522	1088	1094	1098	rVB5	80007	112562	3.01%	0.371%
23	8.610	1106	1109	1114	rVB4	43930	75787	2.02%	0.250%
24	8.675	1116	1120	1123	rVV	67261	72631	1.94%	0.239%
25	8.857	1148	1151	1154	rVB3	41123	50724	1.35%	0.167%
26	8.963	1165	1169	1171	rBV4	57915	67141	1.79%	0.221%
27	8.992	1171	1174	1179	rVB5	86996	118600	3.17%	0.391%
28	9.039	1179	1182	1184	rBV4	36359	40445	1.08%	0.133%
29	9.075	1185	1188	1190	rBV3	65223	75387	2.01%	0.248%
30	9.128	1195	1197	1201	rBV3	47699	50351	1.34%	0.166%
31	9.181	1203	1206	1208	rBV	104456	81428	2.17%	0.268%
32	9.222	1208	1213	1216	rBV	3772096	3745319	100.00%	12.345%
33	9.322	1227	1230	1233	rBV3	64092	74898	2.00%	0.247%
34	9.386	1239	1241	1243	rBV2	57379	58933	1.57%	0.194%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
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Acq On : 6 Oct 2017 22:07
Operator : SJ/JU
Sample : I5516-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.469	1252	1255	1257	rBV2	58581	66679	1.78%	0.220%
36	9.510	1260	1262	1263	rBV	50919	39926	1.07%	0.132%
37	9.610	1277	1279	1284	rVB	138068	144944	3.87%	0.478%
38	9.716	1292	1297	1300	rBV6	76459	147071	3.93%	0.485%
39	9.816	1312	1314	1319	rVB4	49670	66269	1.77%	0.218%
40	9.898	1320	1328	1333	rVV	1255246	1217011	32.49%	4.012%
41	9.945	1333	1336	1339	rVV3	61839	62628	1.67%	0.206%
42	10.110	1362	1364	1369	rVB	53316	62050	1.66%	0.205%
43	10.157	1369	1372	1377	rBV4	90831	133987	3.58%	0.442%
44	10.204	1377	1380	1382	rVV3	77582	96217	2.57%	0.317%
45	10.239	1382	1386	1391	rVV4	146249	221154	5.90%	0.729%
46	10.280	1391	1393	1395	rVV2	66514	65756	1.76%	0.217%
47	10.316	1397	1399	1403	rVB4	80957	77784	2.08%	0.256%
48	10.457	1420	1423	1425	rBV2	84924	78052	2.08%	0.257%
49	10.639	1451	1454	1457	rBV2	80672	100062	2.67%	0.330%
50	10.692	1458	1463	1466	rBV	1958490	1980154	52.87%	6.527%
51	10.792	1478	1480	1485	rVB4	60460	66786	1.78%	0.220%
52	11.239	1553	1556	1557	rBV2	48915	43566	1.16%	0.144%
53	11.257	1557	1559	1563	rVB2	62694	61381	1.64%	0.202%
54	11.386	1577	1581	1584	rBV	1287447	1088729	29.07%	3.589%
55	11.727	1636	1639	1642	rBV	112256	84665	2.26%	0.279%
56	11.910	1667	1670	1679	rVB2	126651	147433	3.94%	0.486%
57	12.692	1800	1803	1810	rVB	62582	67587	1.80%	0.223%
58	12.974	1846	1851	1854	rBV	3232331	3486463	93.09%	11.492%
59	13.557	1947	1950	1953	rBV	196324	150894	4.03%	0.497%
60	13.857	1998	2001	2004	rBV	47942	47609	1.27%	0.157%
61	14.021	2026	2029	2033	rBV	861365	780850	20.85%	2.574%
62	14.857	2168	2171	2174	rVB	43244	41108	1.10%	0.136%
63	15.498	2274	2280	2295	rVB	464778	630763	16.84%	2.079%

Sum of corrected areas: 30337649

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
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Misc :
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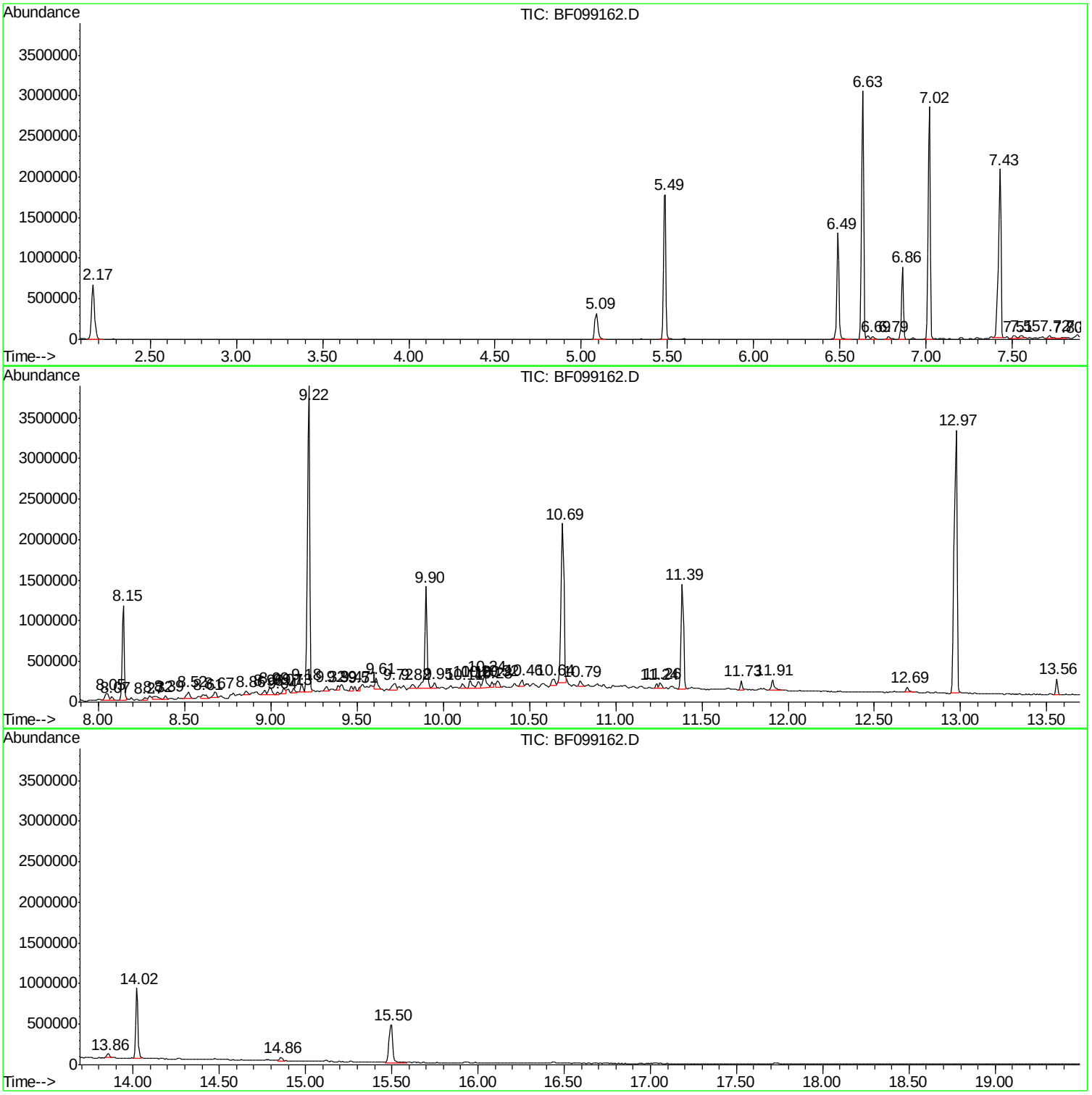
Instrument : BNA_F
ClientSampleId : LIP-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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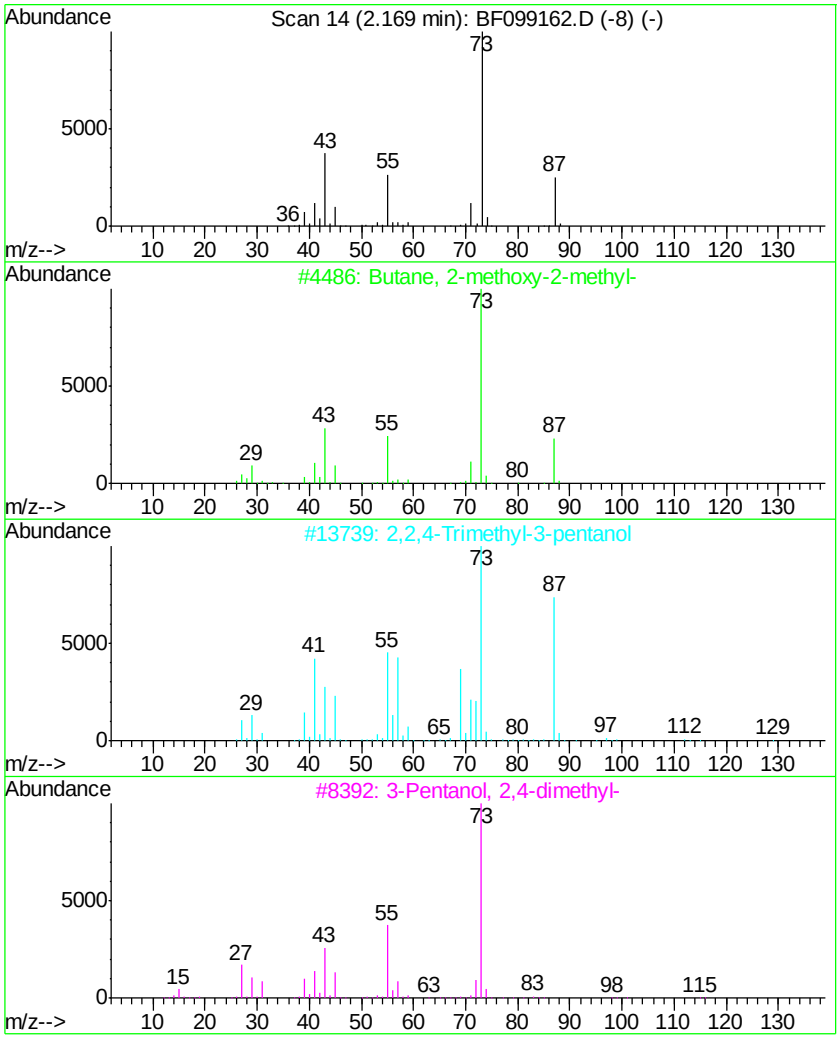
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

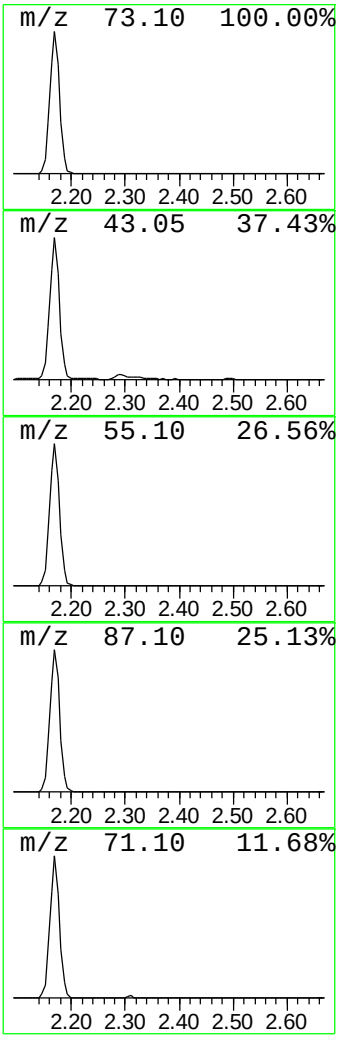
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	23.16 ng	841622	1,4-Dichlorobenzene-d4	6.86

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	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099162.D
Acq On : 6 Oct 2017 22:07
Operator : SJ/JU
Sample : I5516-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

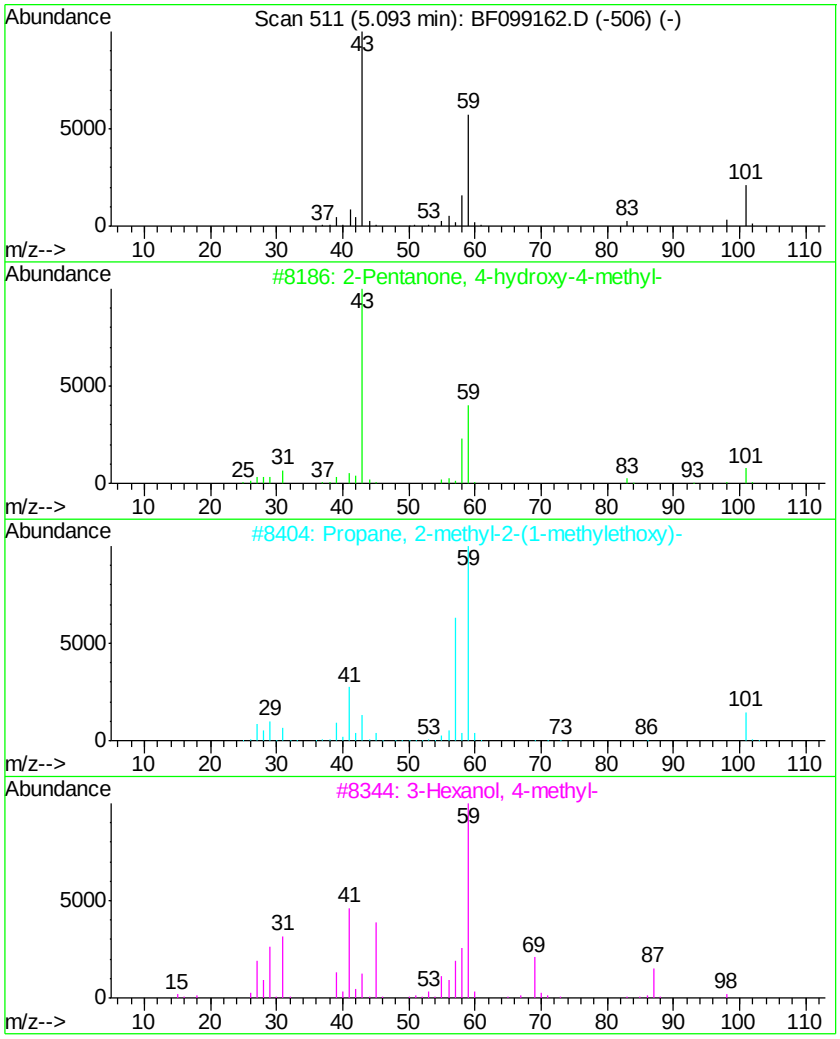
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

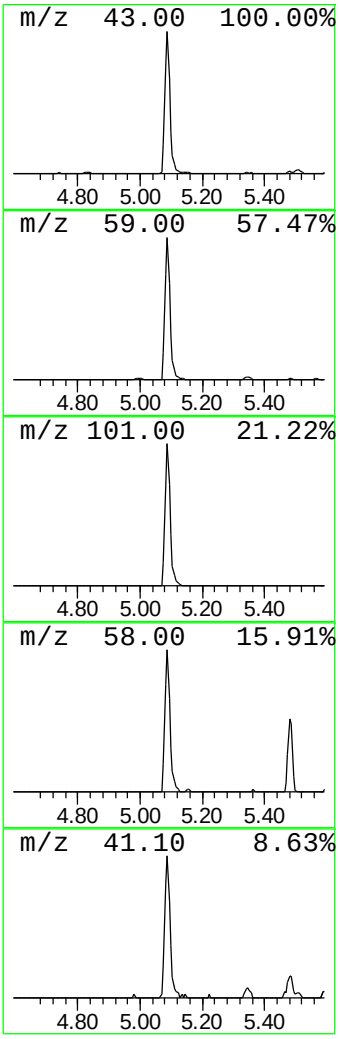
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	9.88 ng	359018	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099162.D
Acq On : 6 Oct 2017 22:07
Operator : SJ/JU
Sample : I5516-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

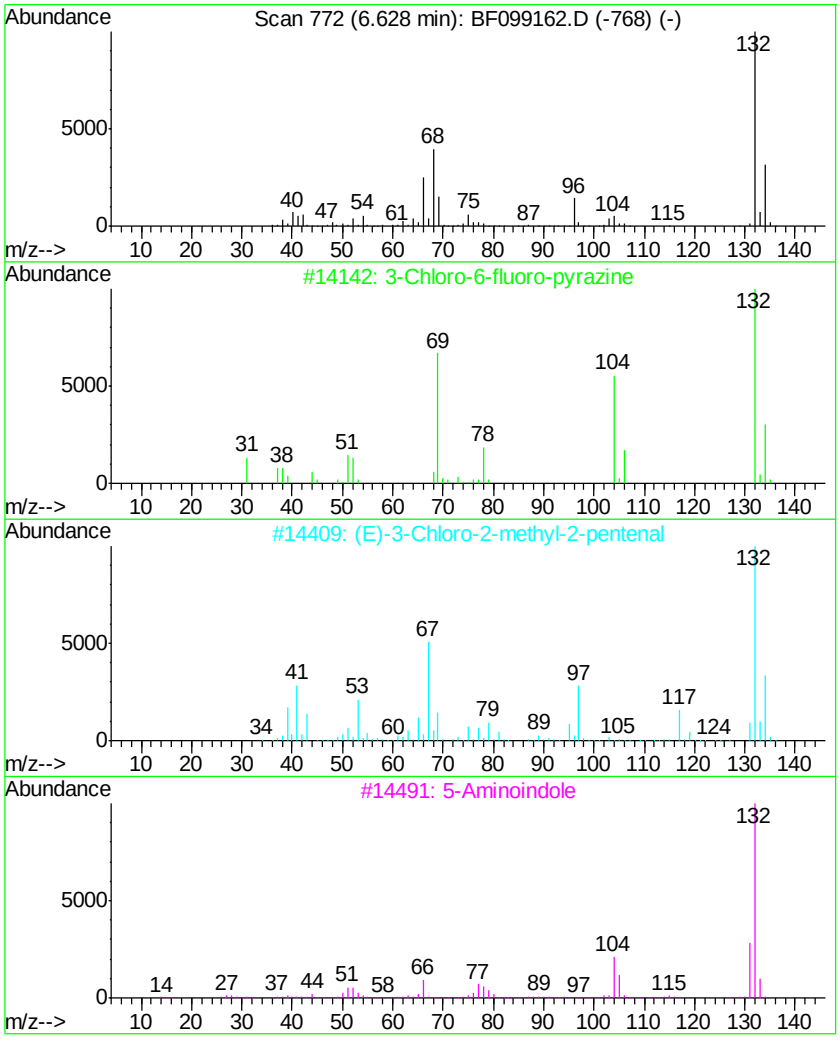
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

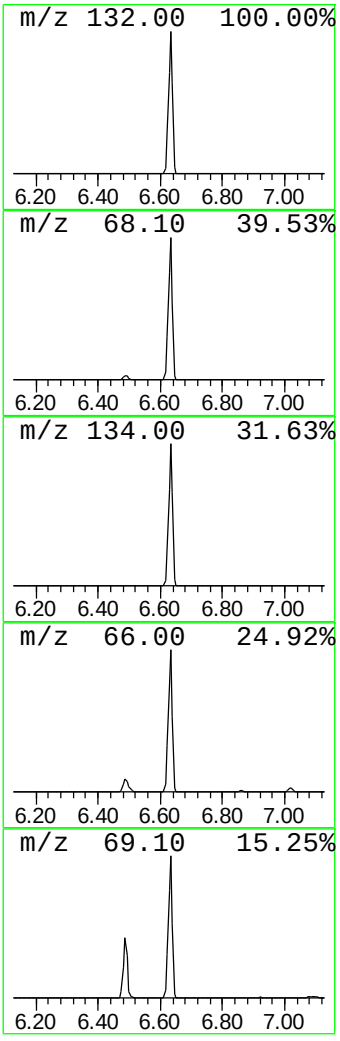
****

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	80.24 ng	2915910	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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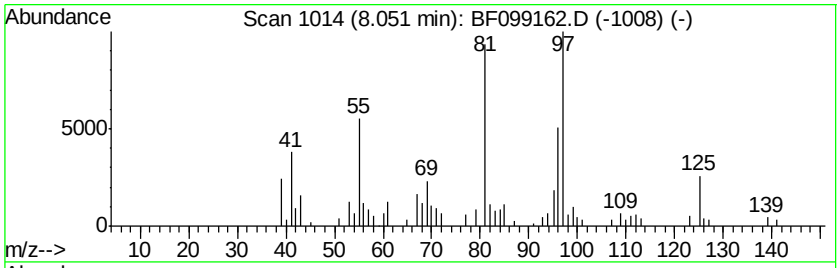
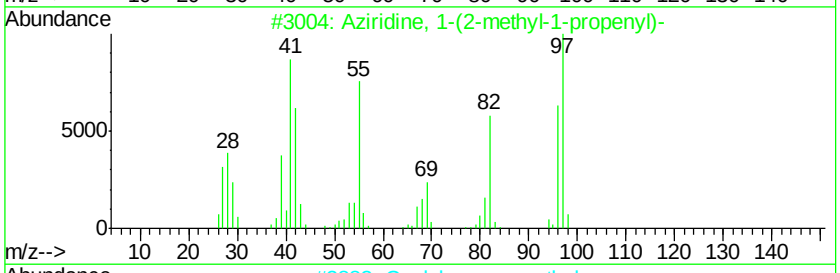
****

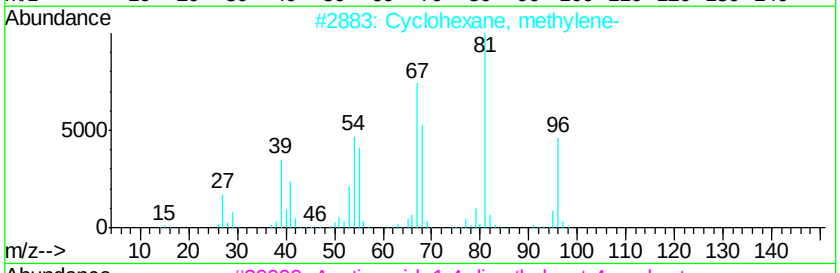
Peak Number 5 unknown8.05 Concentration Rank 12

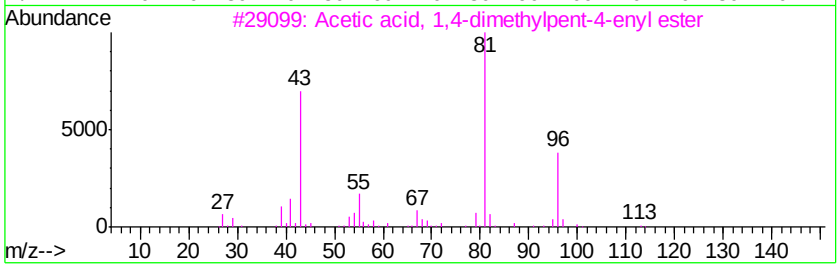
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.05	2.07 ng	108241	Naphthalene-d8	8.15

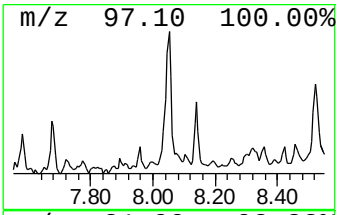
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aziridine, 1-(2-methyl-1-propenyl)-	97	C6H11N	080839-93-6	43
2	Cyclohexane, methylene-	96	C7H12	001192-37-6	43
3	Acetic acid, 1,4-dimethylpent-4-...	156	C9H16O2	1000186-38-5	38
4	1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	38
5	Cyclopropane, trimethylmethylene-	96	C7H12	034462-28-7	38

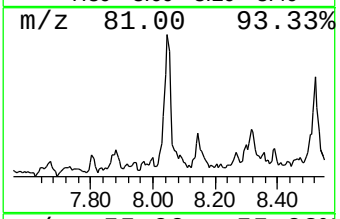


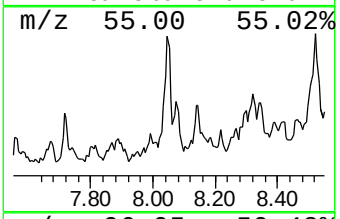


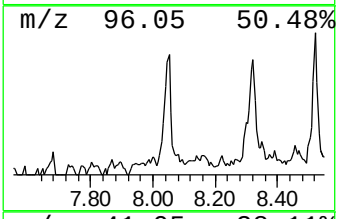


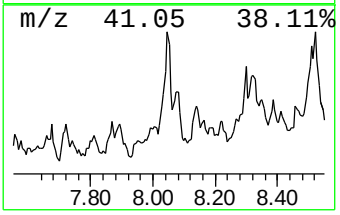












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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

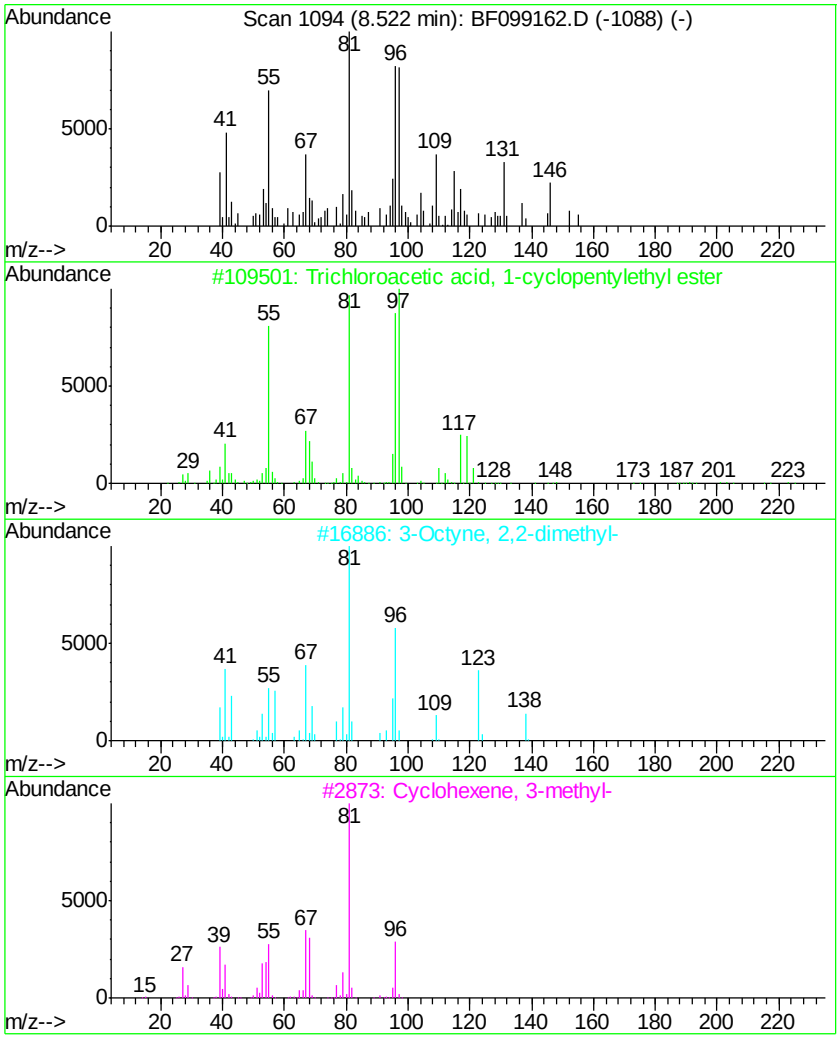
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

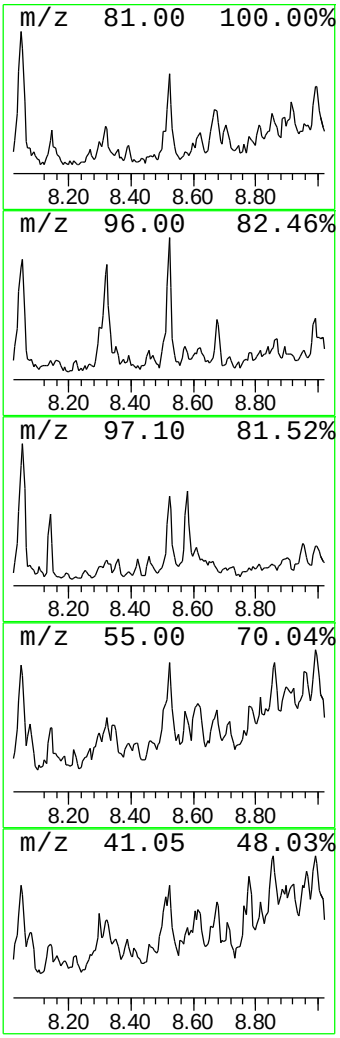
****

Peak Number 6 unknown8.52 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	2.15 ng	112562	Naphthalene-d8	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, 1-cyclopen...	258	C9H13Cl3O2	1000282-57-1	43
2	3-Octyne, 2,2-dimethyl-	138	C10H18	019482-57-6	38
3	Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	38
4	2,4-Hexadiene, 2-methyl-	96	C7H12	028823-41-8	35
5	1,4-Hexadiene, 4-methyl-	96	C7H12	001116-90-1	35





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Data File : BF099162.D
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

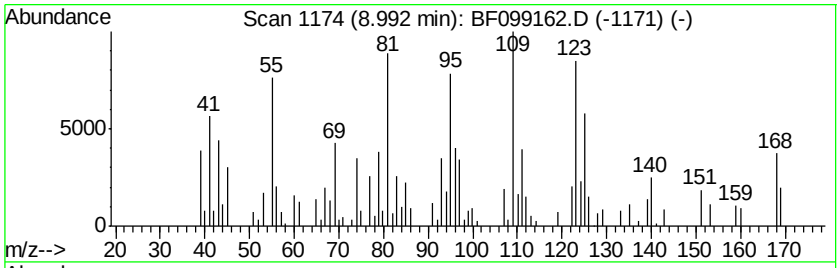
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

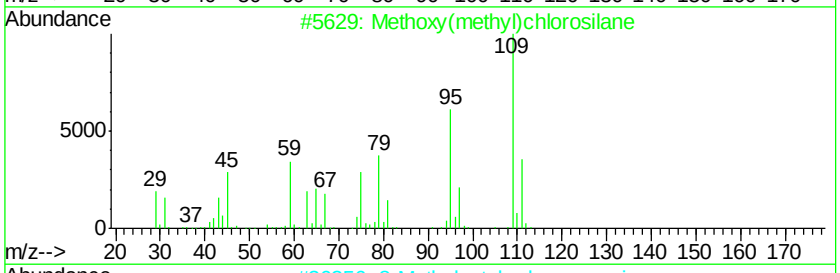
****

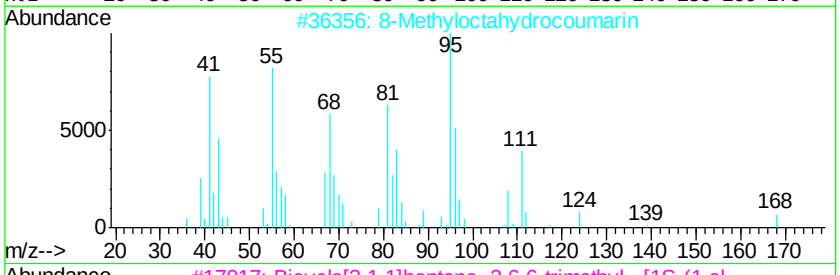
Peak Number 7 unknown8.99 Concentration Rank 9

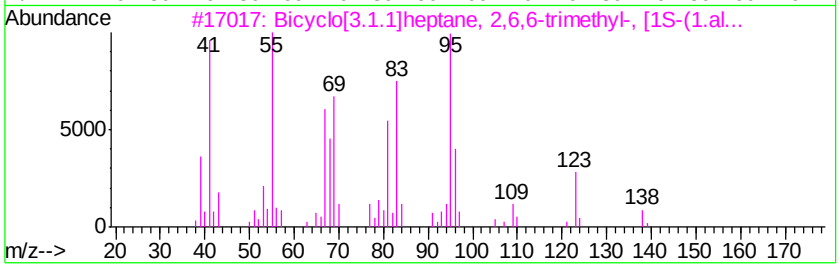
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.99	2.26 ng	118600	Naphthalene-d8	8.15

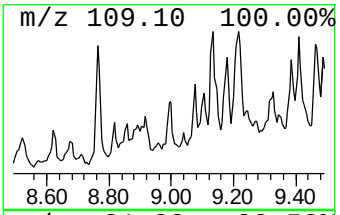
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxy(methyl)chlorosilane	110	C2H7ClOSi	018151-27-4	30
2	8-Methyloctahydrocoumarin	168	C10H16O2	021197-56-8	30
3	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004755-33-3	27
4	1H-Imidazole, 2-ethyl-	96	C5H8N2	001072-62-4	27
5	3-Hydroxymandelic acid	168	C8H8O4	017119-15-2	22

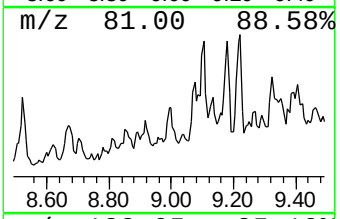


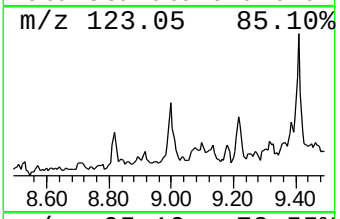


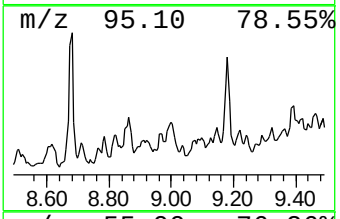


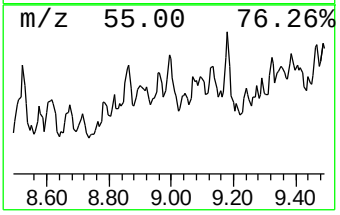












Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
Data File : BF099162.D
Acq On : 6 Oct 2017 22:07
Operator : SJ/JU
Sample : I5516-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

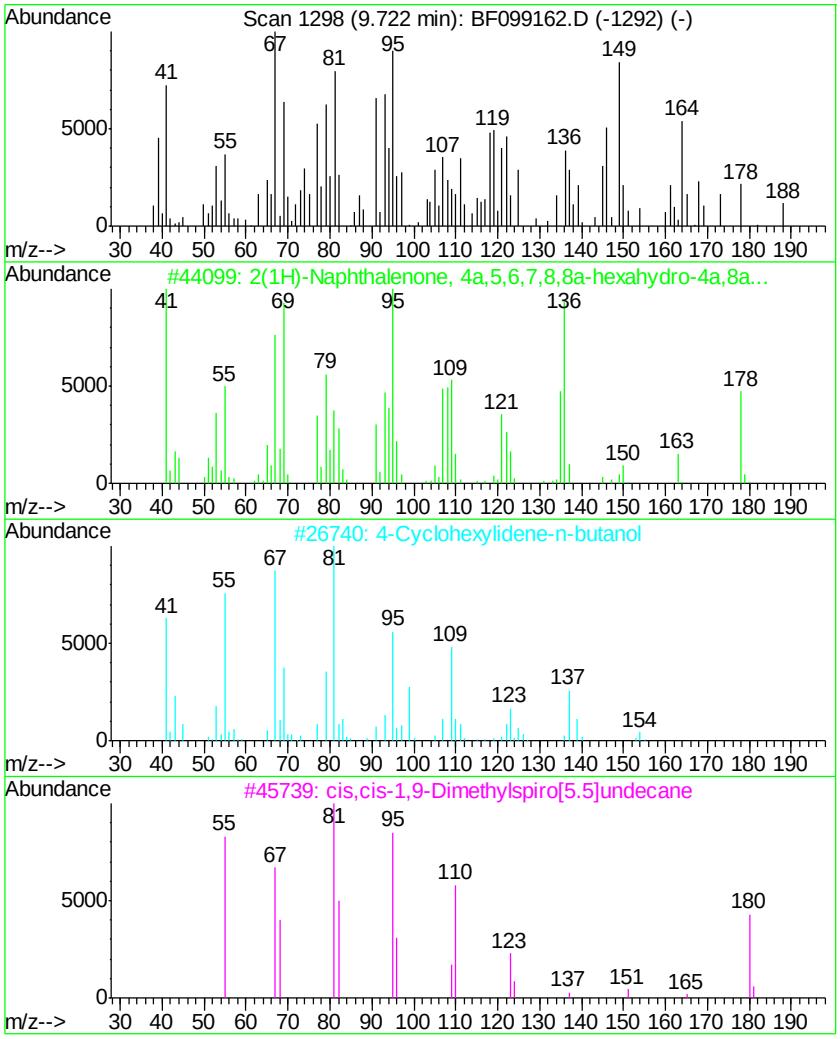
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

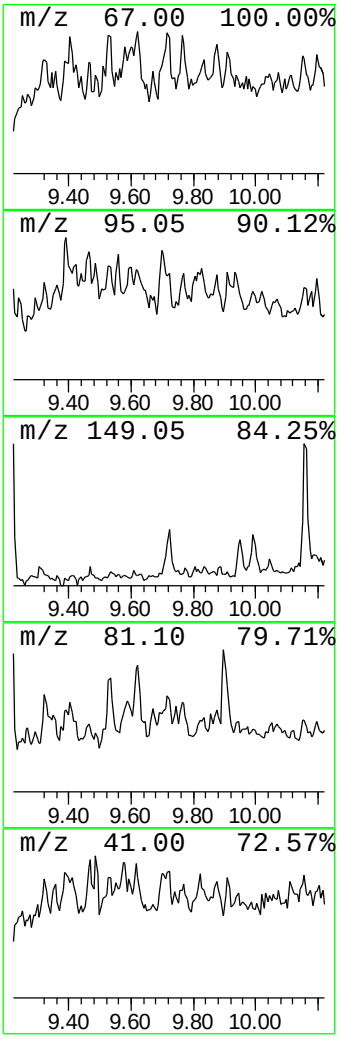
****

Peak Number 8 unknown9.72 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.72	2.42 ng	147071	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Naphthalenone, 4a,5,6,7,8,...	178	C12H18O	013485-66-0	45
2	4-Cyclohexylidene-n-butanol	154	C10H18O	004441-58-1	43
3	cis,cis-1,9-Dimethylspiro[5.5]un...	180	C13H24	1000111-73-4	43
4	1-Methylcycloheptene	110	C8H14	055308-20-8	30
5	Bicyclo[2.2.1]hept-2-en-7-ol	110	C7H10O	053783-87-2	25





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TIC Integration Parameters: LSCINT.P

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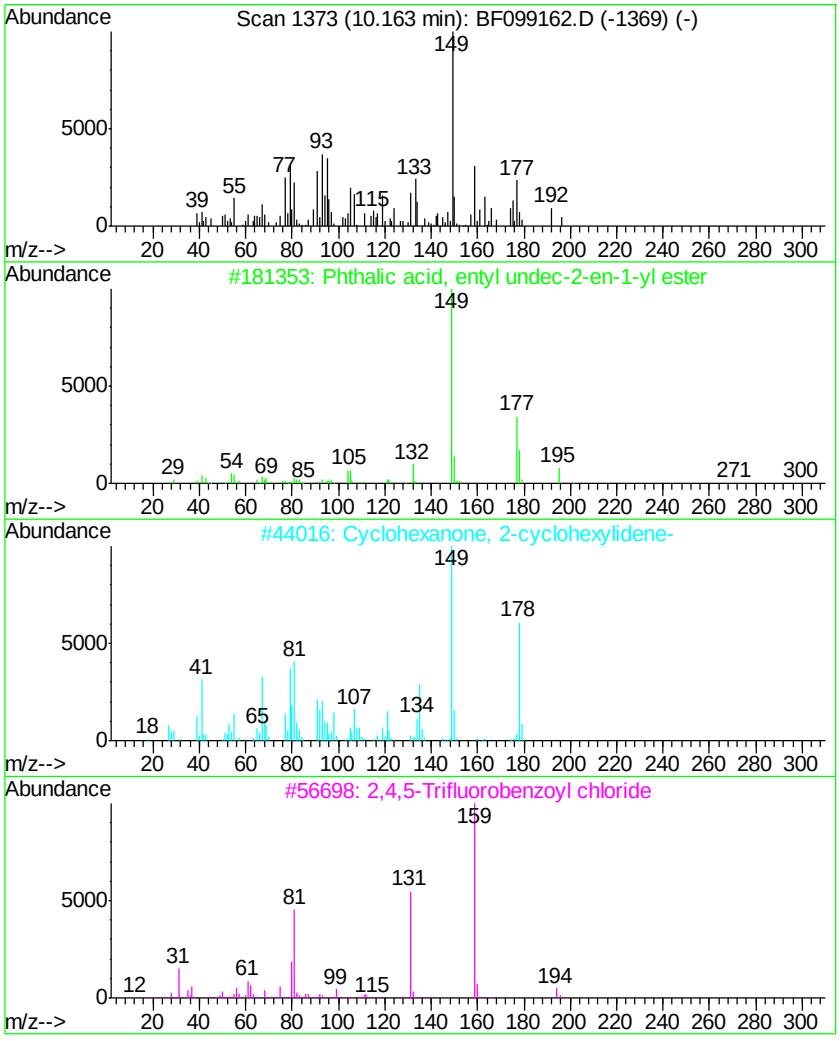
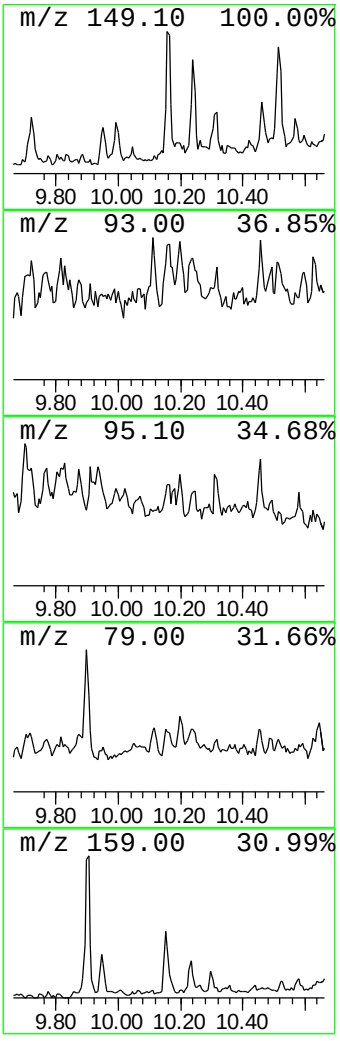
Peak Number 9 unknown10.66 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.16	2.20 ng	133987	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, entyl undec-2-en-...	346	C21H30O4	1000315-41-3	22
2	Cyclohexanone, 2-cyclohexylidene-	178	C12H18O	001011-12-7	20
3	2,4,5-Trifluorobenzoyl chloride	194	C7H2ClF3O	088419-56-1	14
4	Silane, trimethyl(phenylethynyl)-	174	C11H14Si	002170-06-1	11
5	2-Methyl-6-hydroxyquinoline	159	C10H9NO	000613-21-8	11





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Acq On : 6 Oct 2017 22:07
Operator : SJ/JU
Sample : I5516-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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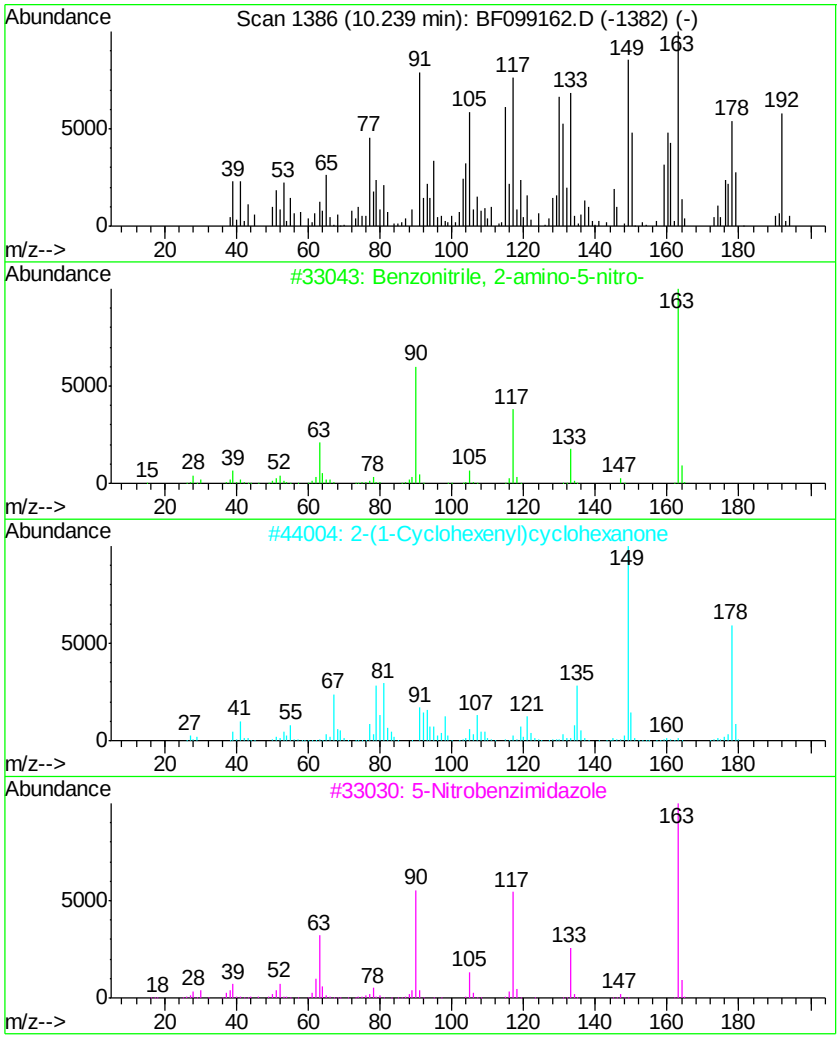
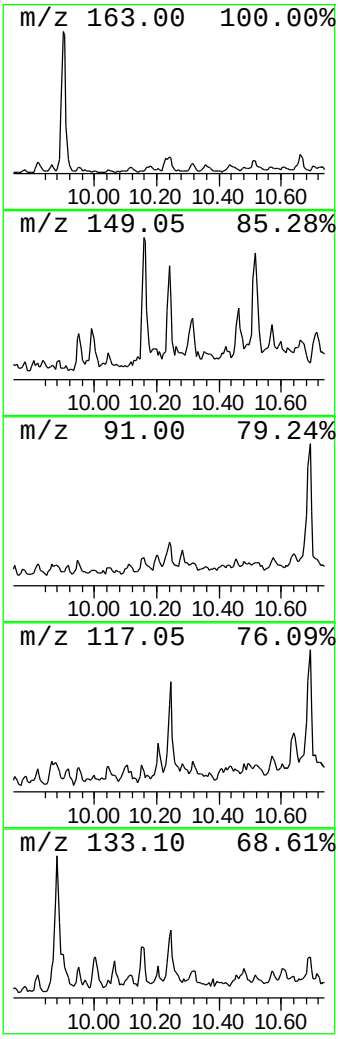
Peak Number 10 unknown10.24 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.24	3.63 ng	221154	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzonitrile, 2-amino-5-nitro-	163	C7H5N3O2	017420-30-3	25
2	2-(1-Cyclohexenyl)cyclohexanone	178	C12H18O	001502-22-3	25
3	5-Nitrobenzimidazole	163	C7H5N3O2	1000229-89-5	25
4	1H-Indene, 2,3-dihydro-5-nitro-	163	C9H9NO2	007436-07-9	18
5	4-Amino-2-nitrobenzonitrile	163	C7H5N3O2	072115-07-2	18





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Sample : I5516-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
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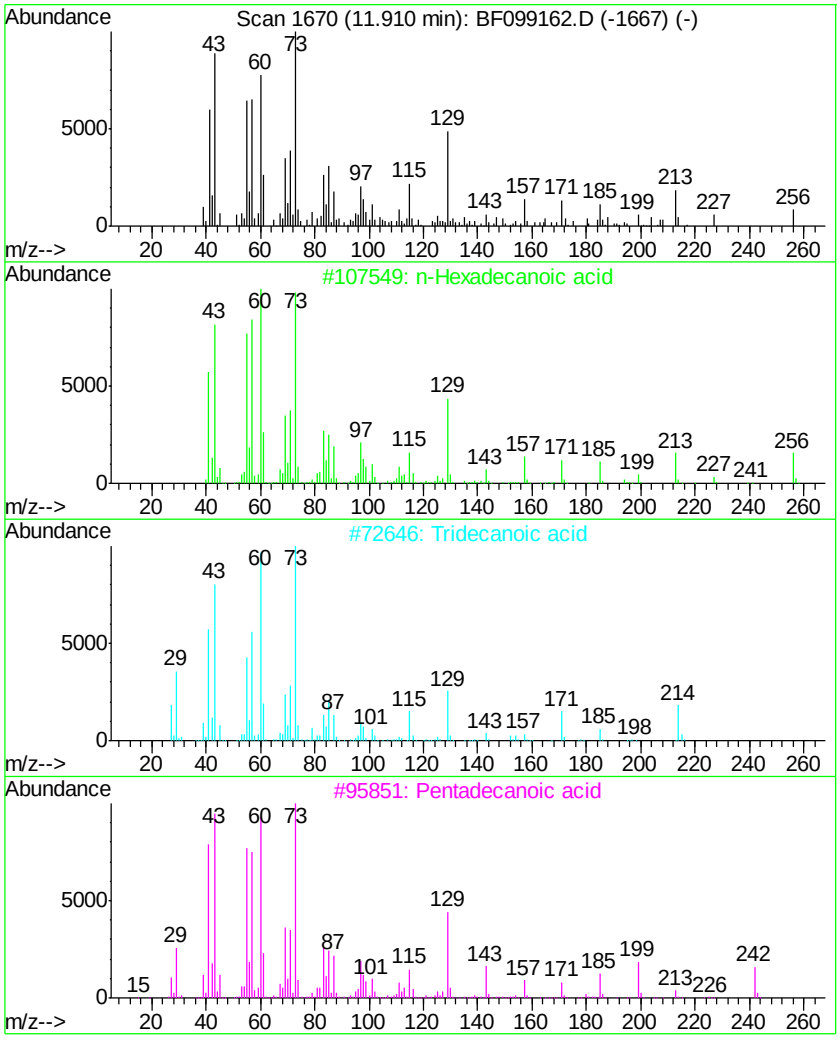
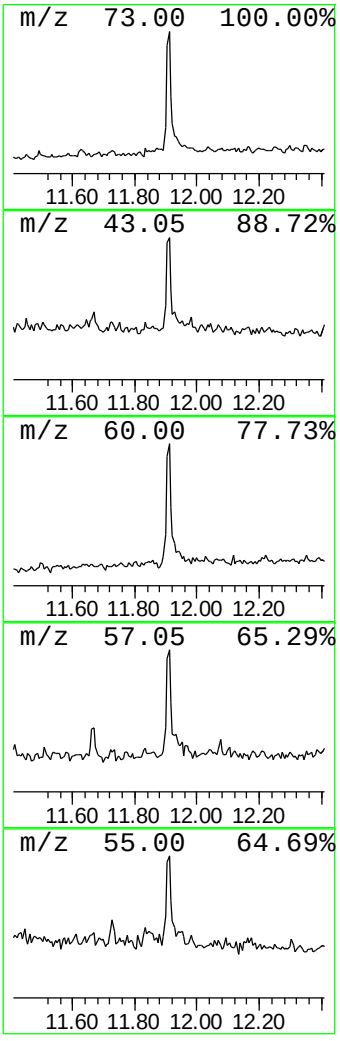
Peak Number 11 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	2.71 ng	147433	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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Data File : BF099162.D
Acq On : 6 Oct 2017 22:07
Operator : SJ/JU
Sample : I5516-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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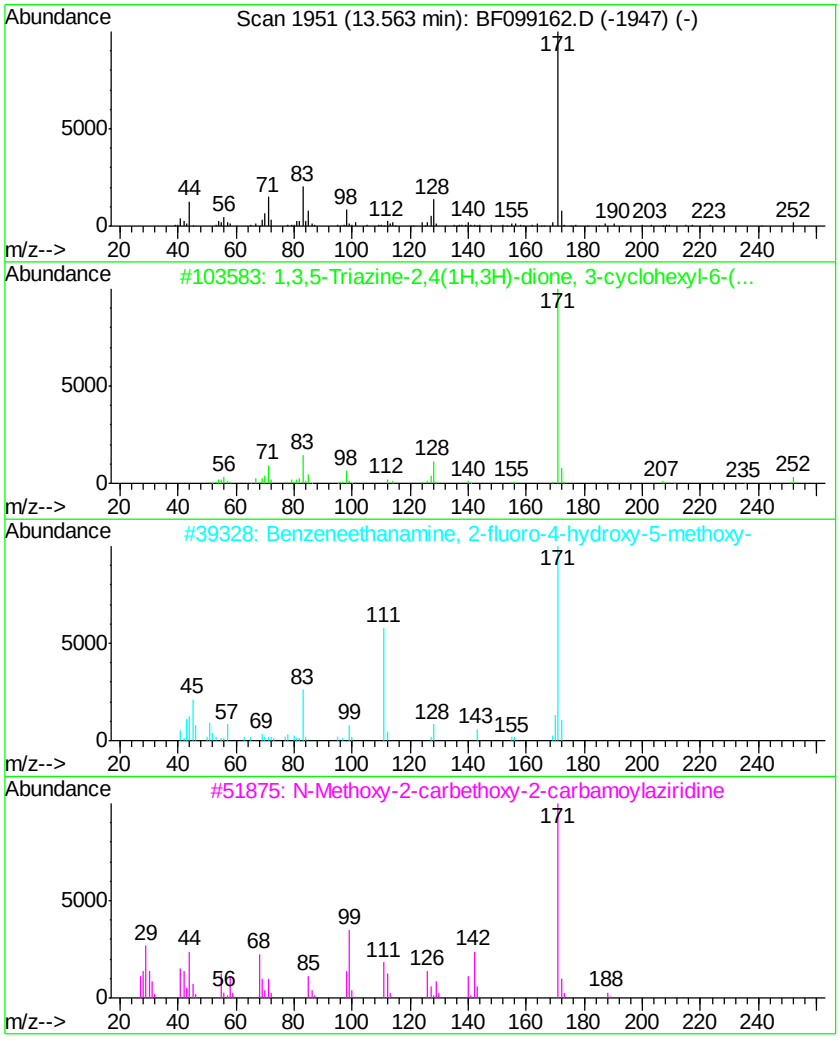
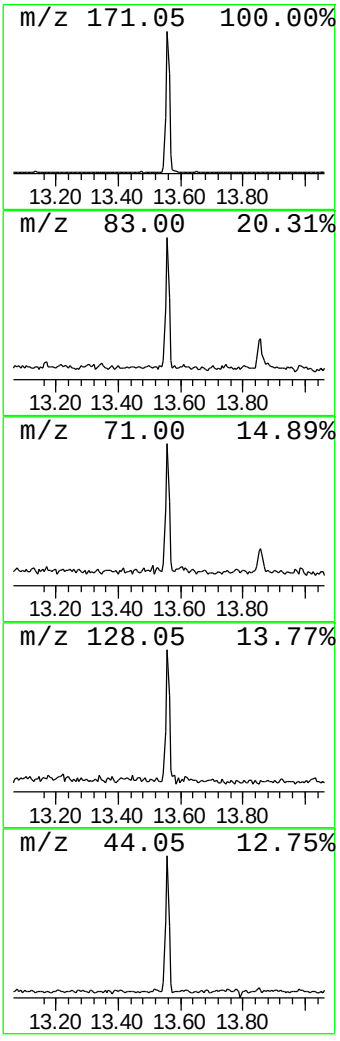
Peak Number 12 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.56	3.86 ng	150894	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4(1H,3H)-dione,...	252	C12H20N4O2	051235-04-2	97
2	Benzeneethanamine, 2-fluoro-4-hy...	171	C8H10FNO2	1000116-43-3	53
3	N-Methoxy-2-carbethoxy-2-carbamo...	188	C7H12N2O4	063859-03-0	38
4	Thiazolo[5,4-d]pyrimidine, 5-chl...	171	C5H2ClN3S	013316-08-0	36
5	Malonic acid, 2,4-dimethylpent-3...	286	C16H30O4	1000349-01-3	33





Tentatively Identified Compound (LSC) summary

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Data File : BF099162.D
Acq On : 6 Oct 2017 22:07
Operator : SJ/JU
Sample : I5516-04
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Instrument : BNA_F
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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...	2.17	23.2	ng	841622	1	6.86	726839	20.0
2-Pentanone, 4-hy...	5.09	9.9	ng	359018	1	6.86	726839	20.0
unknown6.63	6.63	80.2	ng	2915910	1	6.86	726839	20.0
unknown8.05	8.05	2.1	ng	108241	2	8.15	1047720	20.0
unknown8.52	8.52	2.1	ng	112562	2	8.15	1047720	20.0
unknown8.99	8.99	2.3	ng	118600	2	8.15	1047720	20.0
unknown9.72	9.72	2.4	ng	147071	3	9.90	1217010	20.0
unknown10.66	10.16	2.2	ng	133987	3	9.90	1217010	20.0
unknown10.24	10.24	3.6	ng	221154	3	9.90	1217010	20.0
n-Hexadecanoic acid	11.91	2.7	ng	147433	4	11.39	1088730	20.0
1,3,5-Triazine-2,...	13.56	3.9	ng	150894	5	14.02	780850	20.0