LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102149.D
Acq On : 17 Jan 2018 14:57
Operator : SJ/JU
Sample : J1144-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IGW-1

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-BF010918.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	3.710	268	276	282	rBV	1584514	2358280	77.51%	7.605%
2	4.922	477	482	490	rVB	160473	212774	6.99%	0.686%
3	5.334	546	552	555	rVB	2714443	2859836	93.99%	9.222%
4	6.357	721	726	731	rVB	2828333	2972201	97.68%	9.584%
5	6.486	744	748	752	rBV	3046589	2970454	97.63%	9.579%
6	6.545	755	758	764	rVB3	36728	34977	1.15%	0.113%
7	6.722	784	788	791	rBV	1082038	914665	30.06%	2.949%
8	6.875	810	814	817	rBV	2610688	2209270	72.61%	7.124%
9	7.286	876	884	887	rBV	1974366	1828957	60.11%	5.898%
10	8.004	1001	1006	1015	rBV	1389129	1297516	42.64%	4.184%
11	8.516	1087	1093	1097	rBV	484651	447124	14.70%	1.442%
12	8.557	1097	1100	1104	rVB	43973	34824	1.14%	0.112%
13	8.845	1145	1149	1157	rBV	189643	217049	7.13%	0.700%
14	9.080	1183	1189	1192	rBV	3508131	3042663	100.00%	9.812%
15	9.433	1246	1249	1252	rVB	297119	257859	8.47%	0.832%
16	9.475	1252	1256	1259	rVB	267379	216671	7.12%	0.699%
17	9.757	1299	1304	1307	rBV	1400580	1290266	42.41%	4.161%
18	10.469	1421	1425	1428	rBV	85034	67802	2.23%	0.219%
19	10.545	1433	1438	1441	rBV	2076046	1938291	63.70%	6.250%
20	11.239	1551	1556	1559	rBV	1316896	1221084	40.13%	3.938%
21	11.768	1642	1646	1648	rBV	134756	141273	4.64%	0.456%
22	12.486	1765	1768	1771	rVB	98466	79493	2.61%	0.256%
23	12.704	1802	1805	1807	rBV	85958	79792	2.62%	0.257%
24	12.821	1820	1825	1828	rBV	2804543	2634057	86.57%	8.494%
25	13.715	1974	1977	1984	rVB	171262	176976	5.82%	0.571%
26	13.868	1999	2003	2007	rVB	912459	817079	26.85%	2.635%
27	15.280	2239	2243	2247	rBV	553776	689684	22.67%	2.224%

Sum of corrected areas: 31010917

LSC Report - Integrated Chromatogram

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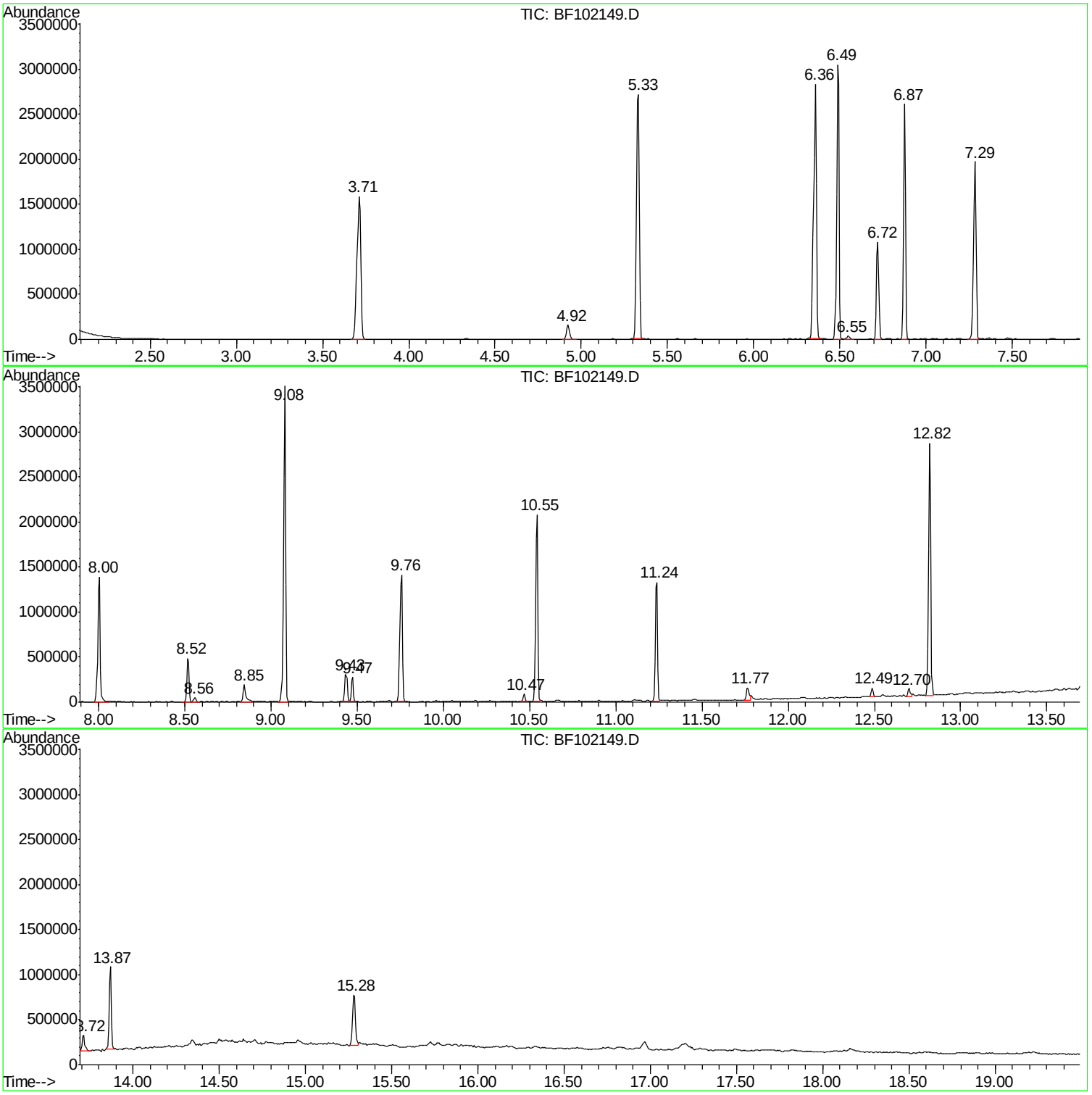
Operator : SJ/JU
Sample : J1144-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IGW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102149.D
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Operator : SJ/JU
Sample : J1144-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IGW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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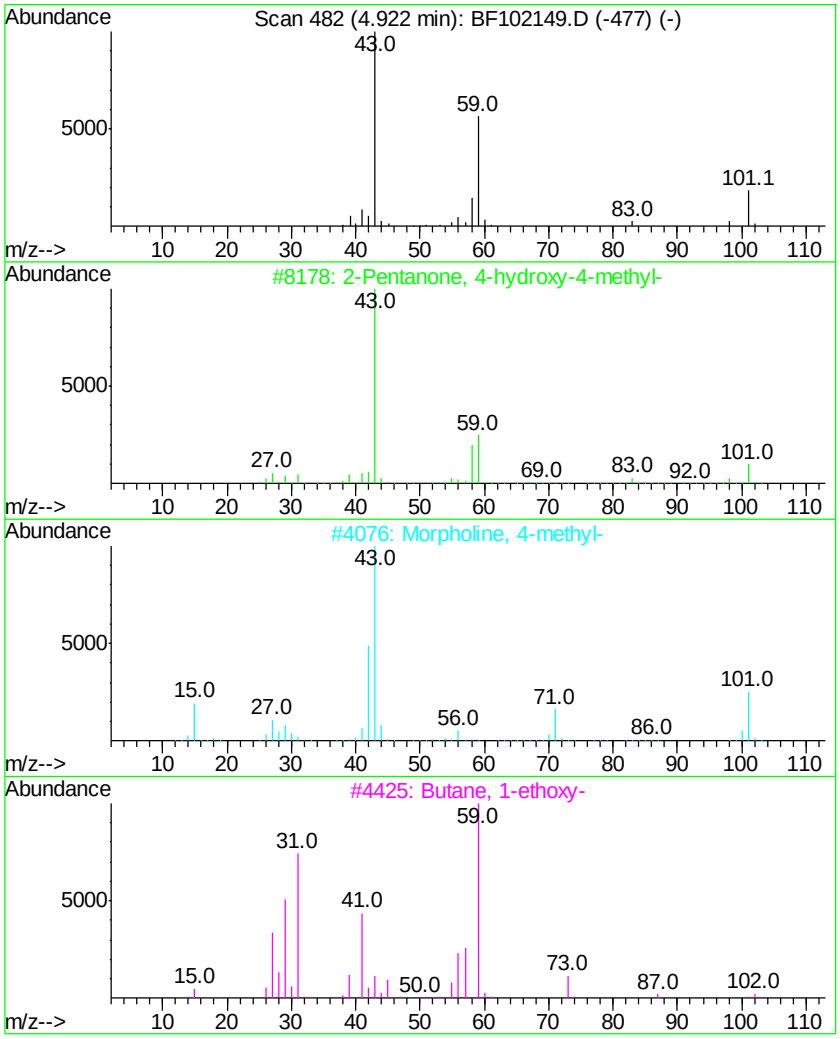
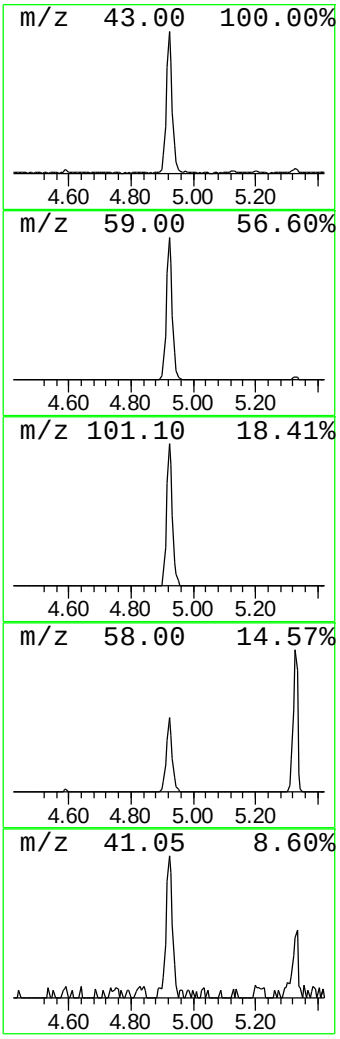
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	4.65 ng	212774	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Diacetamide	101	C4H7NO2	000625-77-4	9





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Sample : J1144-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IGW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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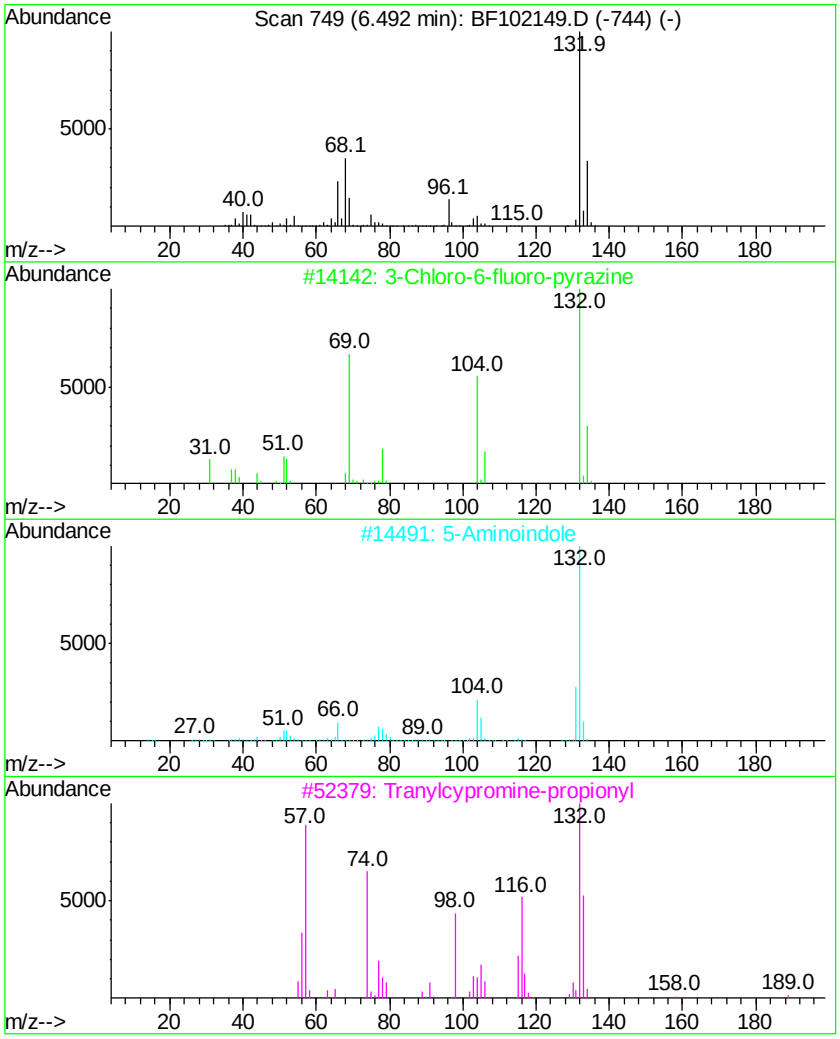
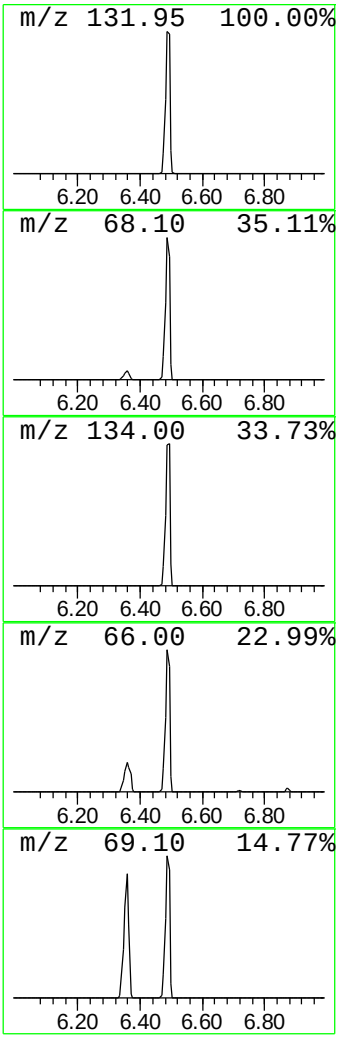
Peak Number 3 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	64.95 ng	2970450	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
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Acq On : 17 Jan 2018 14:57
Operator : SJ/JU
Sample : J1144-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IGW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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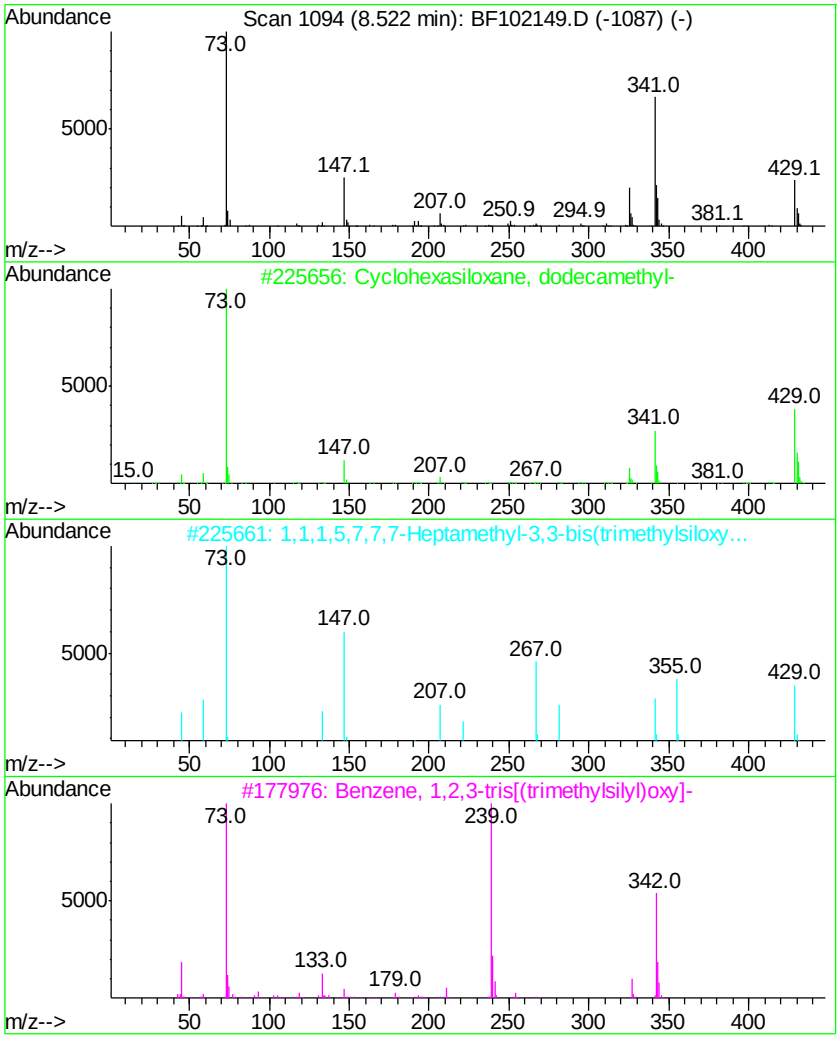
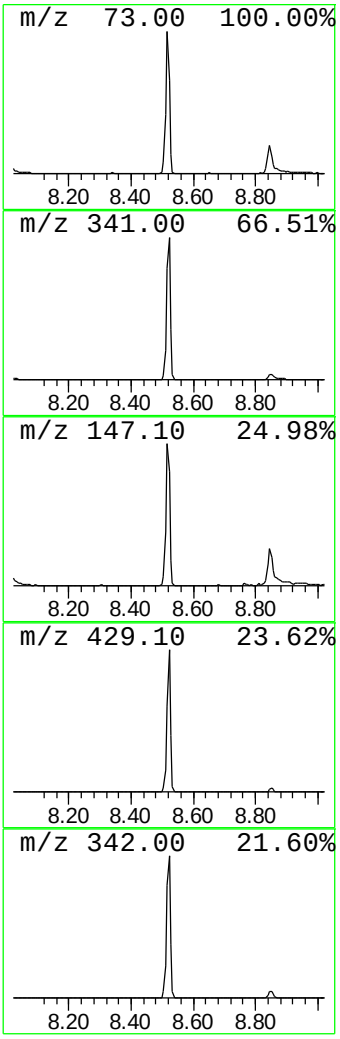
Peak Number 5 Cyclohexasiloxane, dodecame... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	6.89 ng	447124	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexasiloxane, dodecamethyl-	444	C12H36O6Si6	000540-97-6	91
2	1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	32
3	Benzene, 1,2,3-tris[(trimethylsi...	342	C15H30O3Si3	017864-23-2	22
4	Guaifenesin di-tms derivative	342	C16H30O4Si2	107966-19-8	17
5	17-Epi-trenbolone, trimethylsily...	342	C21H30O2Si	1000293-11-0	14





Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102149.D
Acq On : 17 Jan 2018 14:57
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Sample : J1144-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IGW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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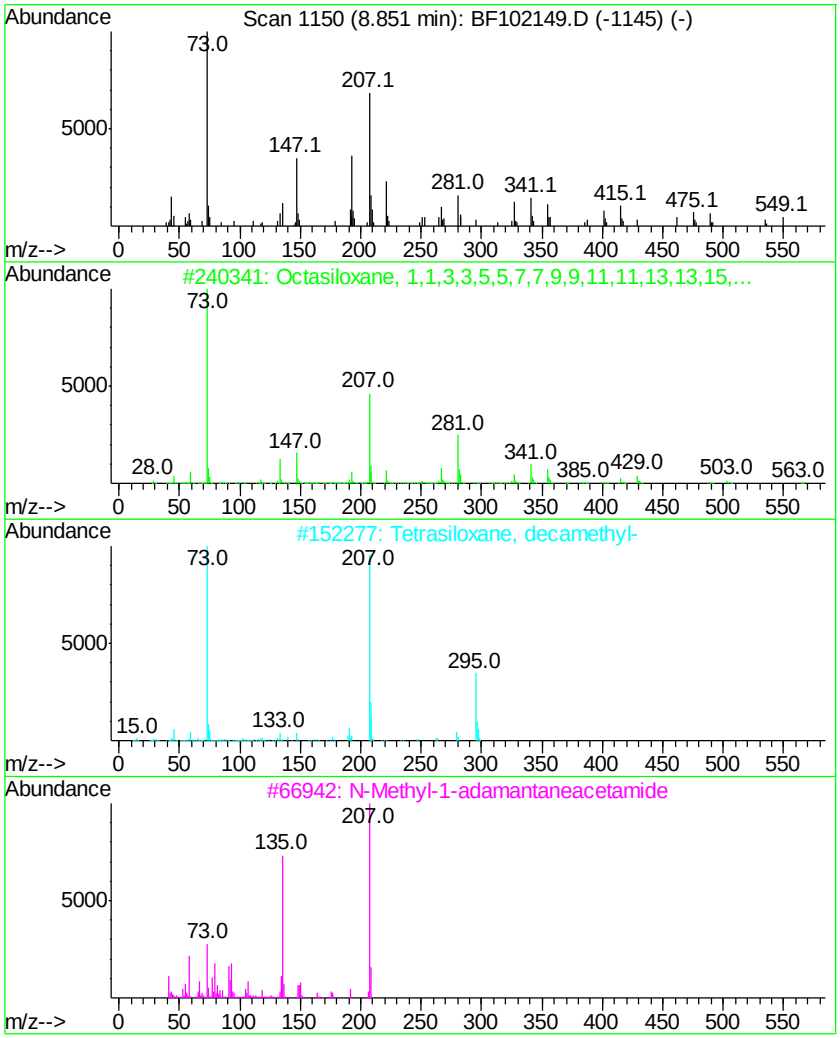
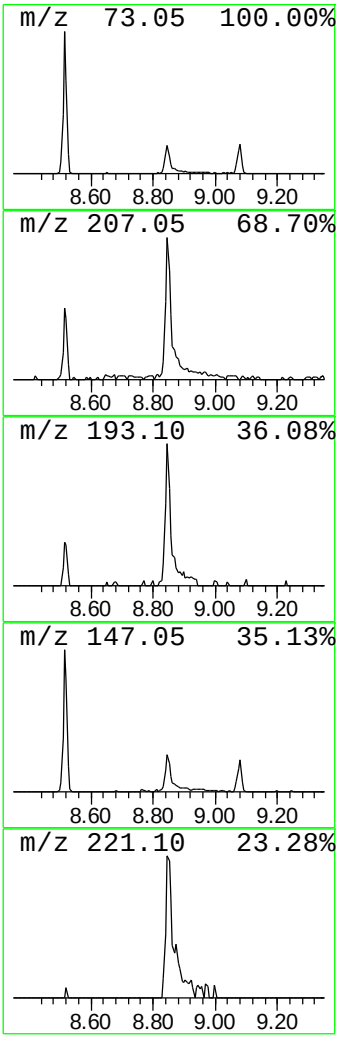
Peak Number 6 unknown8.85 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.85	3.35 ng	217049	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octasiloxane, 1,1,3,3,5,5,7,7,9,...	578	C16H50O7Si8	019095-24-0	37
2	Tetrasiloxane, decamethyl-	310	C10H30O3Si4	000141-62-8	35
3	N-Methyl-1-adamantaneacetamide	207	C13H21NO	031897-93-5	30
4	Propanamide, N-(4-methoxyphenyl)...	207	C12H17NO2	056619-94-4	27
5	Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	27





Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
Data File : BF102149.D
Acq On : 17 Jan 2018 14:57
Operator : SJ/JU
Sample : J1144-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IGW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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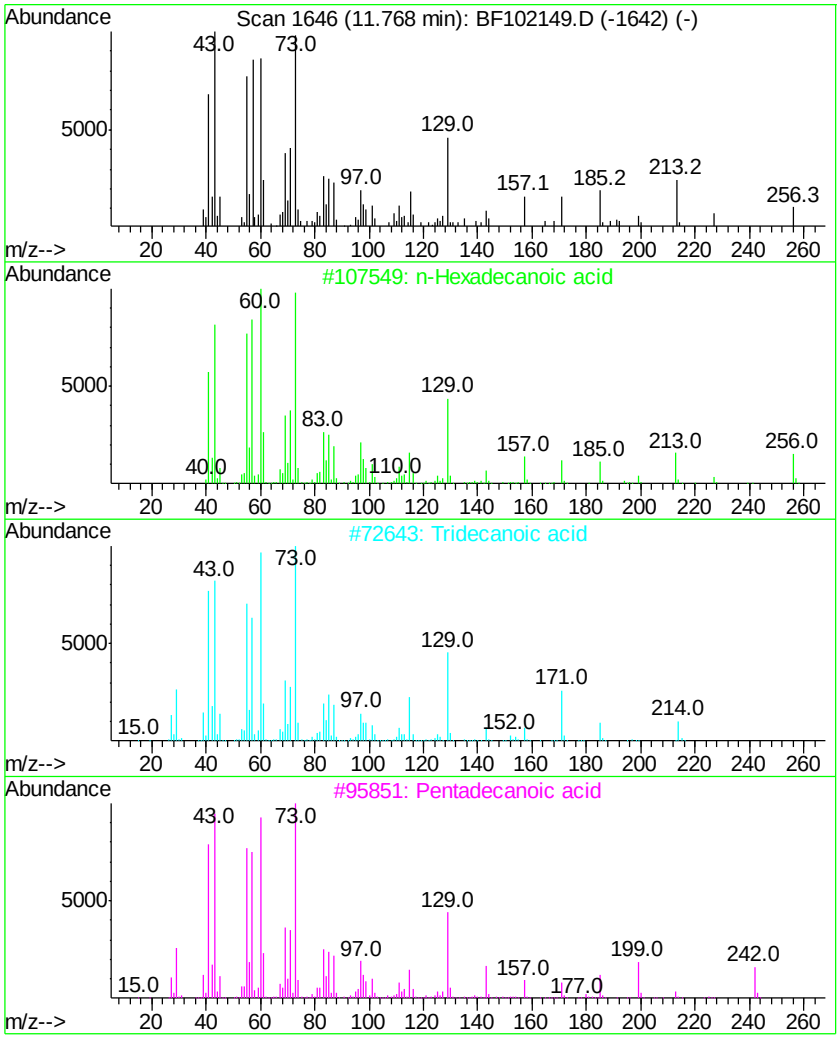
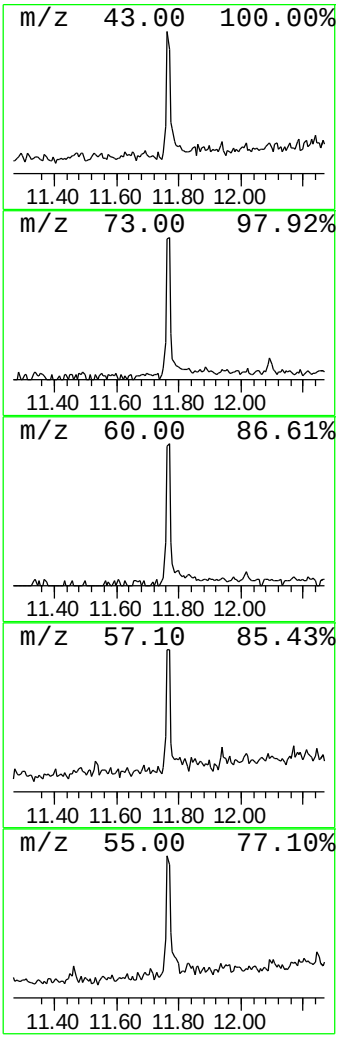
Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	2.31 ng	141273	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47





Library Search Compound Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF011718\
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Operator : SJ/JU
Sample : J1144-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IGW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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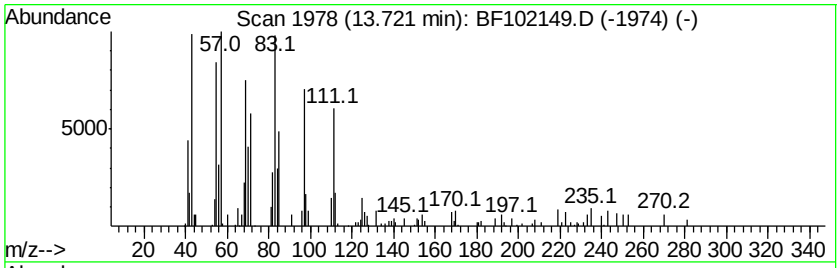
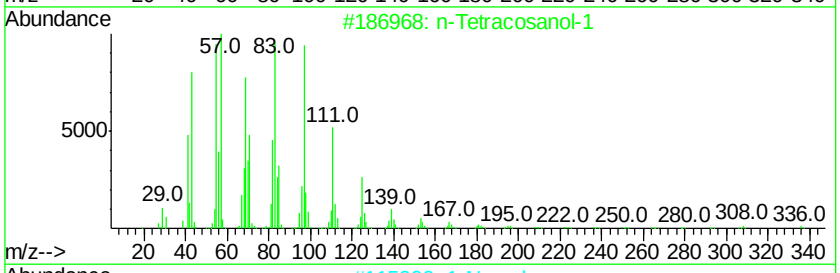
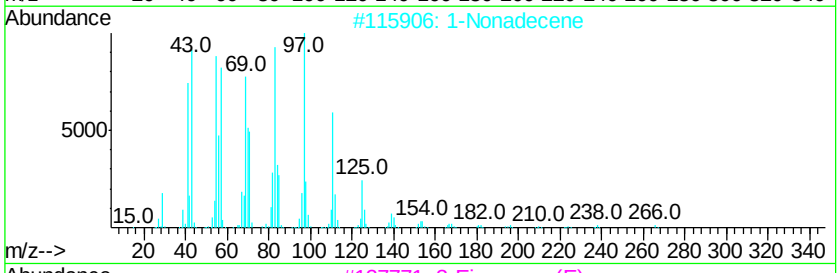
Peak Number 8 n-Tetracosanol-1 Concentration Rank 6

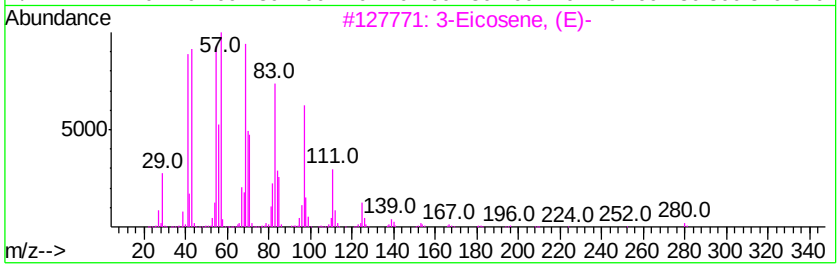
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.33 ng	176976	Chrysene-d12	13.87

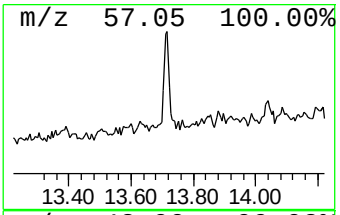
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87

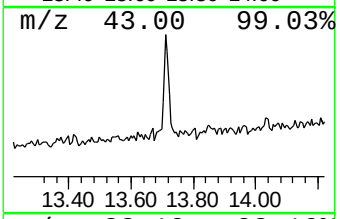


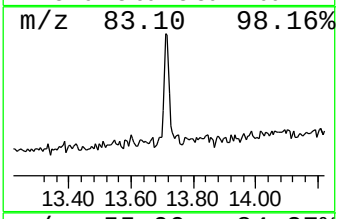


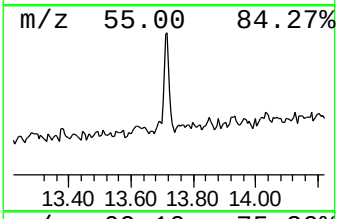


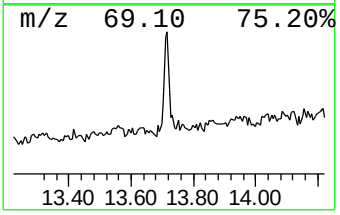












Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	4.7	ng	212774	1	6.72	914665	20.0
unknown6.49	6.49	65.0	ng	2970450	1	6.72	914665	20.0
Cyclohexasiloxane...	8.52	6.9	ng	447124	2	8.00	1297520	20.0
unknown8.85	8.85	3.4	ng	217049	2	8.00	1297520	20.0
n-Hexadecanoic acid	11.77	2.3	ng	141273	4	11.24	1221080	20.0
n-Tetracosanol-1	13.72	4.3	ng	176976	5	13.87	817079	20.0