LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072518\
Data File : BF107655.D
Acq On : 25 Jul 2018 14:26
Operator : JU/SJ
Sample : J4124-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11-S

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-BF072018.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	5.213	484	489	507	rBV	550741	842399	15.28%	1.677%
2	5.601	551	555	581	rBV	3528734	5075068	92.07%	10.102%
3	6.601	720	725	744	rBV	3415743	5199465	94.33%	10.350%
4	6.742	744	749	772	rVB	4452131	5356611	97.18%	10.663%
5	6.966	783	787	809	rVB	1189760	1516827	27.52%	3.019%
6	7.125	809	814	836	rBV	3635312	4247541	77.06%	8.455%
7	7.531	879	883	906	rBV	2624367	3543732	64.29%	7.054%
8	8.248	1001	1005	1022	rBV	1656398	1911617	34.68%	3.805%
9	9.325	1181	1188	1203	rBV	5098301	5512229	100.00%	10.972%
10	9.713	1250	1254	1265	rBV	283336	276157	5.01%	0.550%
11	10.007	1300	1304	1323	rVB	2029800	1959690	35.55%	3.901%
12	10.801	1435	1439	1452	rBV	3088562	3581435	64.97%	7.129%
13	10.889	1452	1454	1460	rVB2	42643	64132	1.16%	0.128%
14	11.501	1554	1558	1567	rBV	1760014	2027289	36.78%	4.035%
15	12.007	1641	1644	1656	rBV3	213564	275109	4.99%	0.548%
16	12.719	1762	1765	1773	rBV	168079	179516	3.26%	0.357%
17	12.948	1799	1804	1811	rBV2	134132	211002	3.83%	0.420%
18	13.089	1823	1828	1839	rBV	4408705	4378939	79.44%	8.716%
19	13.636	1918	1921	1924	rBV2	78707	76209	1.38%	0.152%
20	13.966	1974	1977	1987	rBV	236374	308379	5.59%	0.614%
21	14.154	2004	2009	2019	rBV	1339707	1622430	29.43%	3.230%
22	14.283	2028	2031	2034	rBV	100167	74882	1.36%	0.149%
23	14.589	2081	2083	2086	rBV	85806	84717	1.54%	0.169%
24	14.913	2135	2138	2142	rBV	74605	77201	1.40%	0.154%
25	14.989	2148	2151	2156	rVB	246802	269249	4.88%	0.536%
26	15.265	2195	2198	2203	rVB2	84839	114435	2.08%	0.228%
27	15.683	2264	2269	2281	rBV2	885902	1451235	26.33%	2.889%

Sum of corrected areas: 50237495

LSC Report - Integrated Chromatogram

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Misc :
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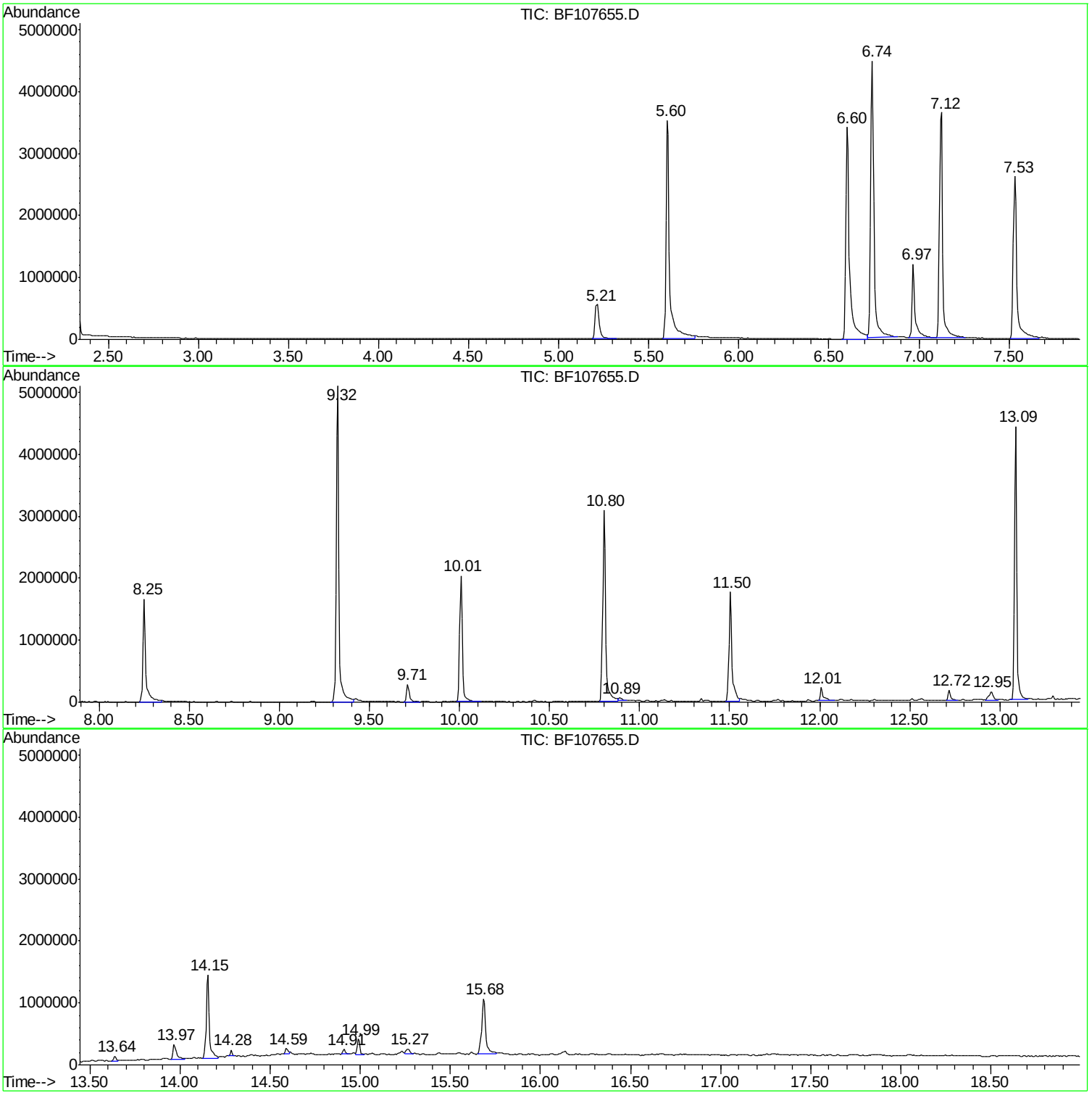
Instrument : BNA_F
ClientSampleId : TP-11-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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

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Misc :
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ClientSampleId : TP-11-S

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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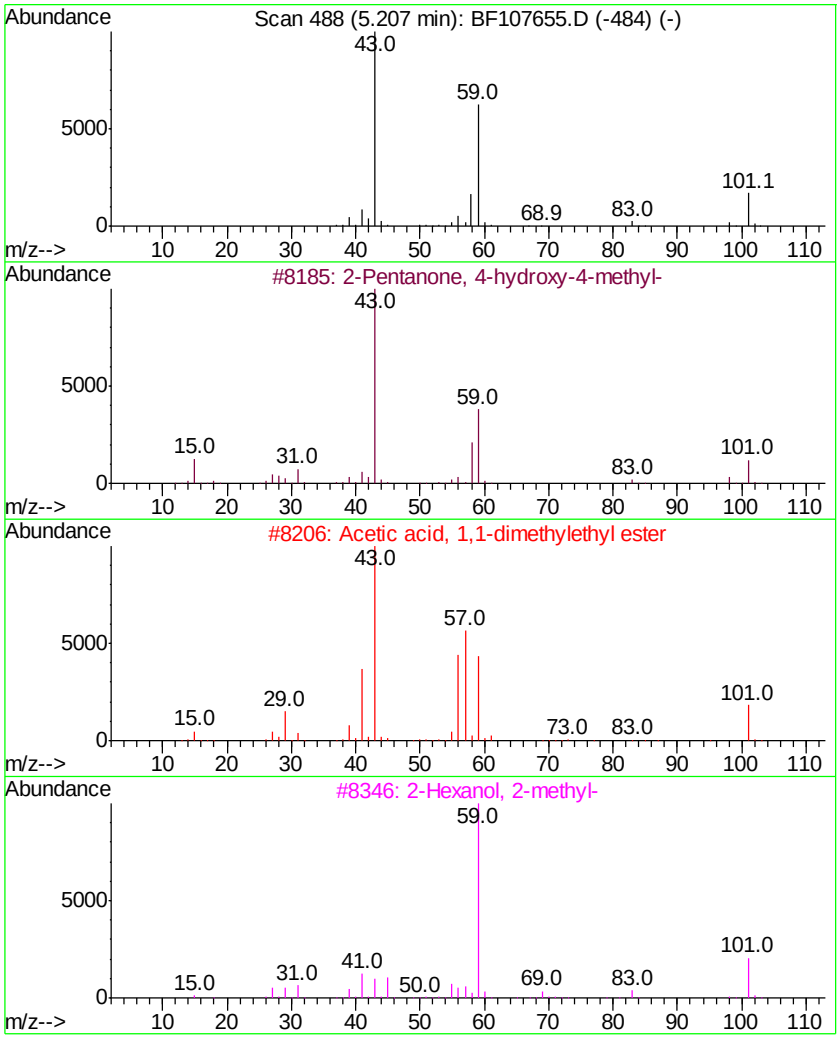
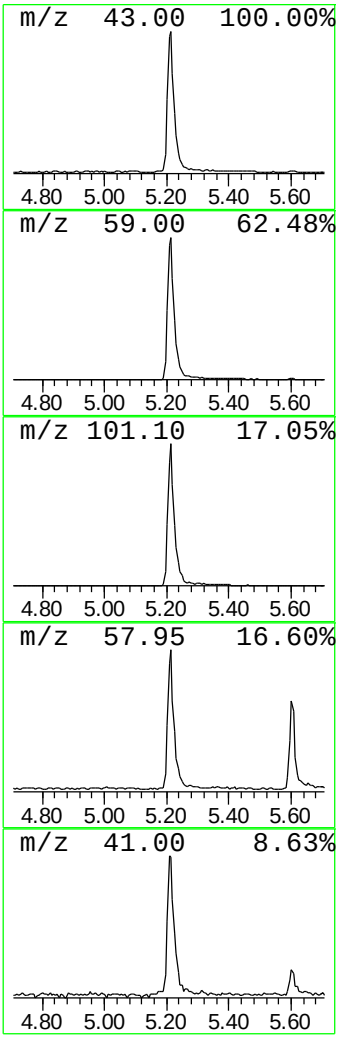
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	11.11 ng	842399	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : TP-11-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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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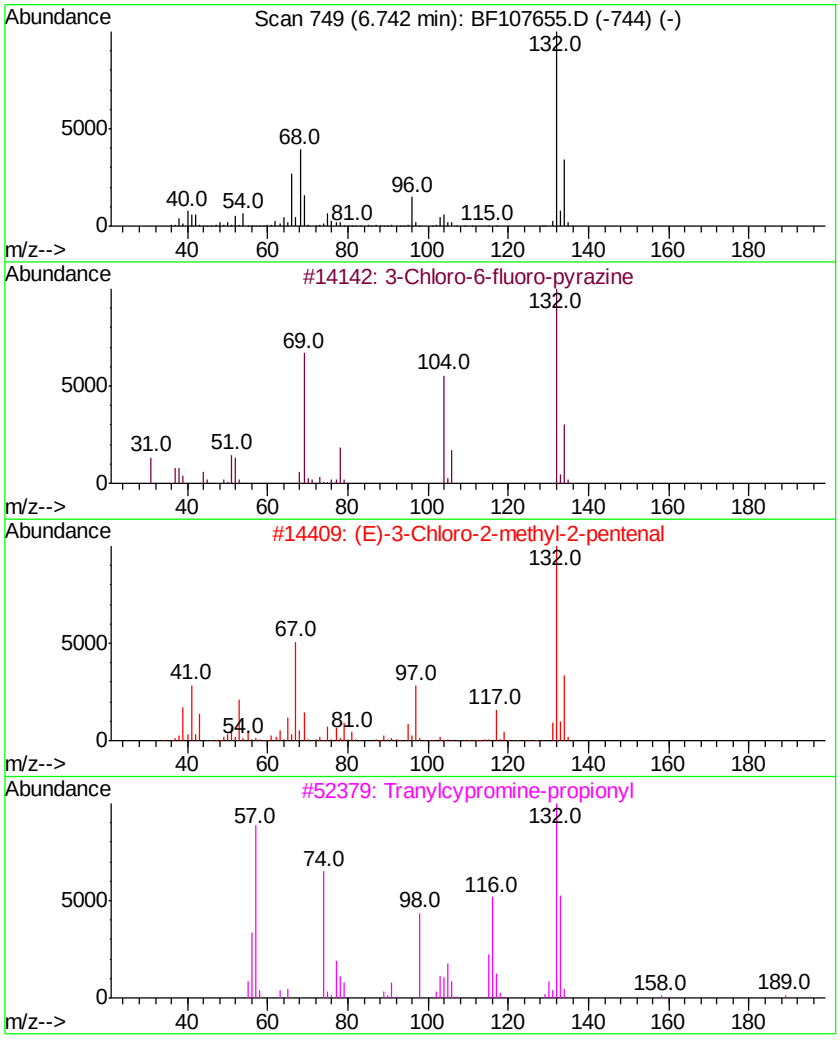
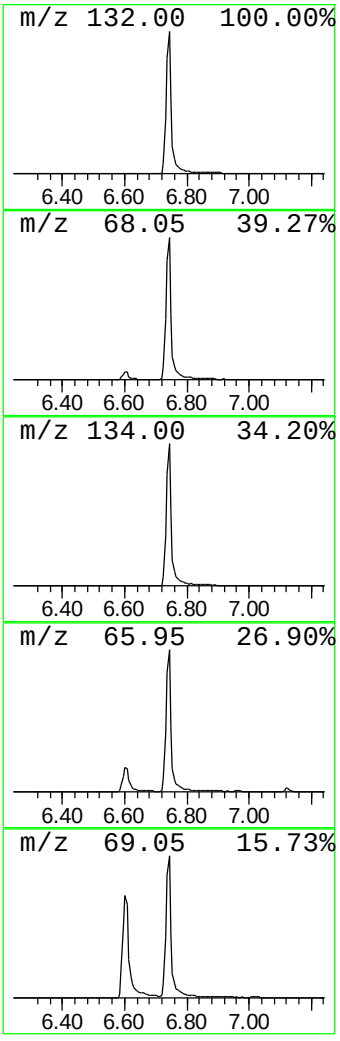
Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	70.63 ng	5356610	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11-S

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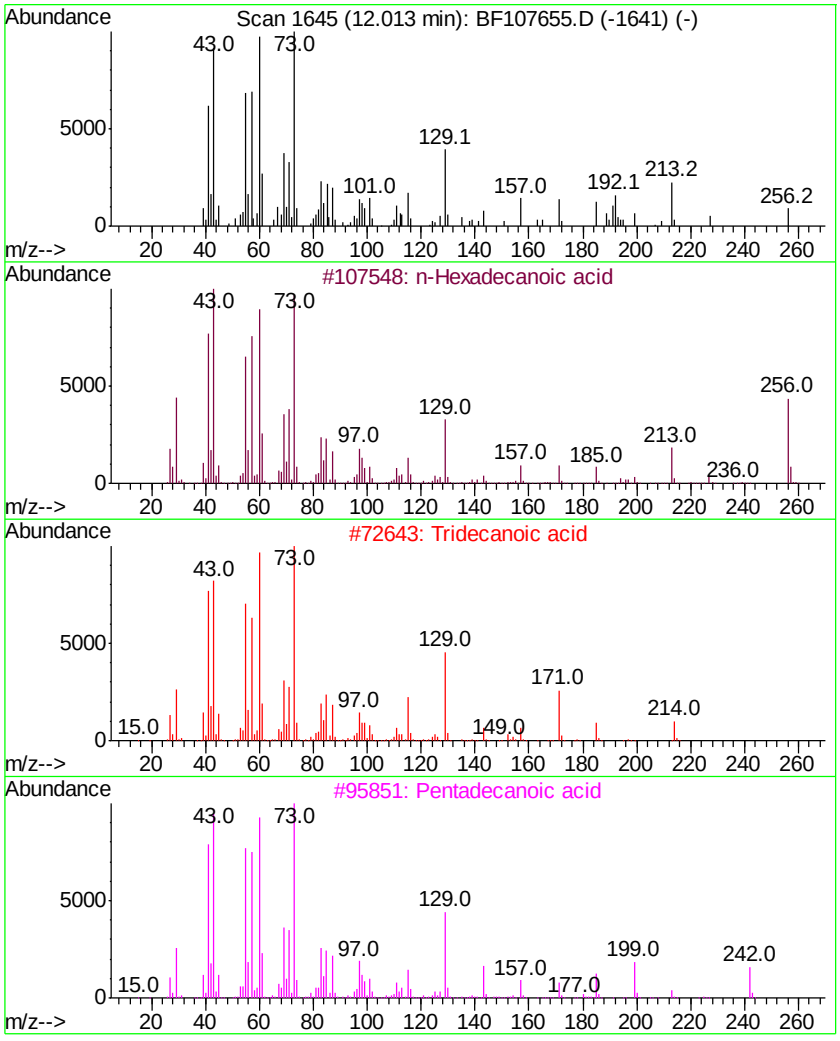
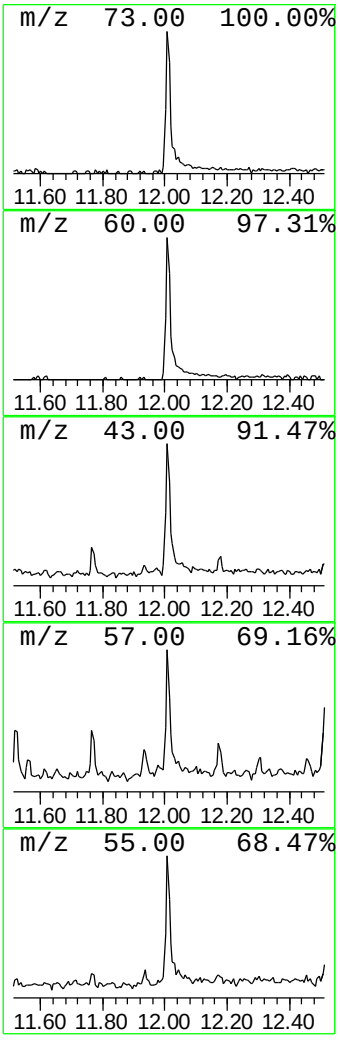
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.71 ng	275109	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





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Sample : J4124-03
Misc :
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Instrument : BNA_F
ClientSampleId : TP-11-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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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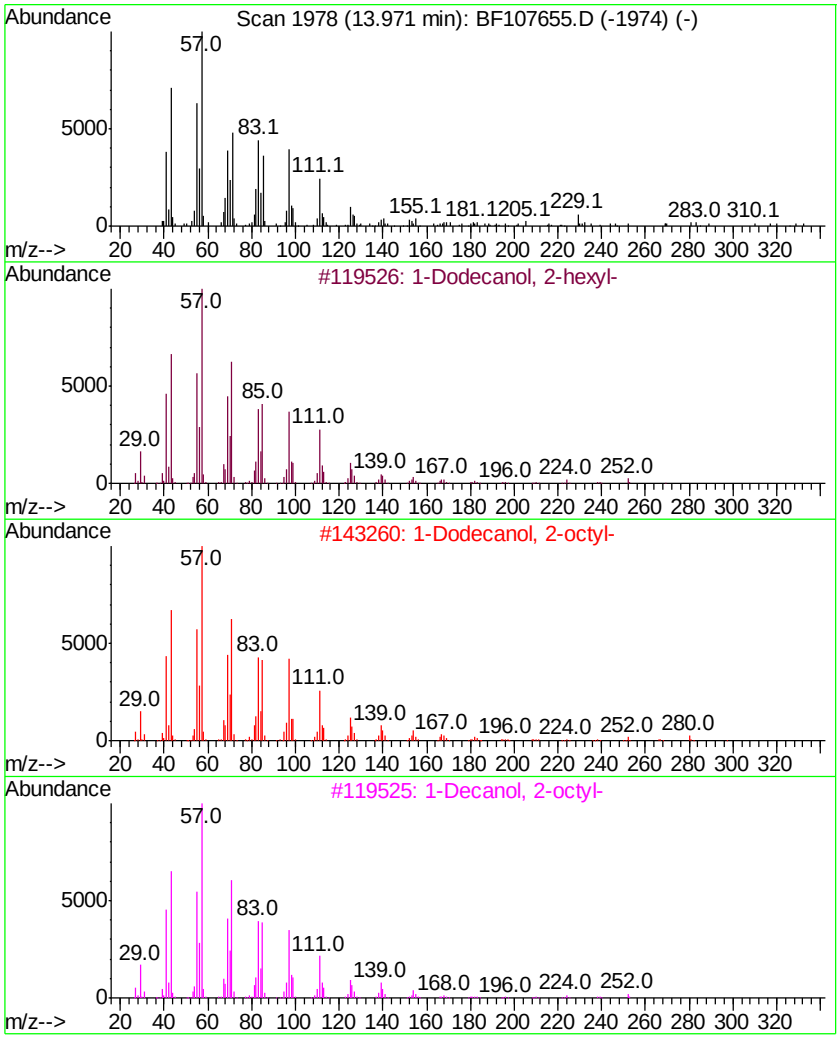
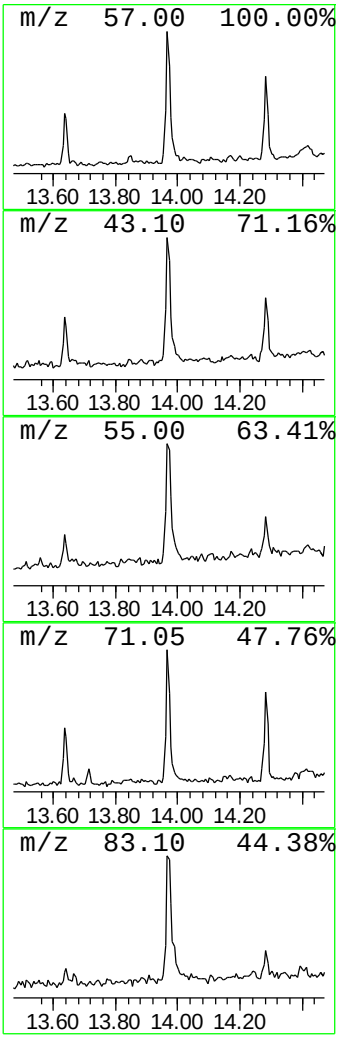
Peak Number 6 1-Dodecanol, 2-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	3.80 ng	308379	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	91
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
3	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	91
4	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	91
5	Tetradecane, 1-chloro-	232	C14H29Cl	002425-54-9	74





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Misc :
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Instrument : BNA_F
ClientSampleId : TP-11-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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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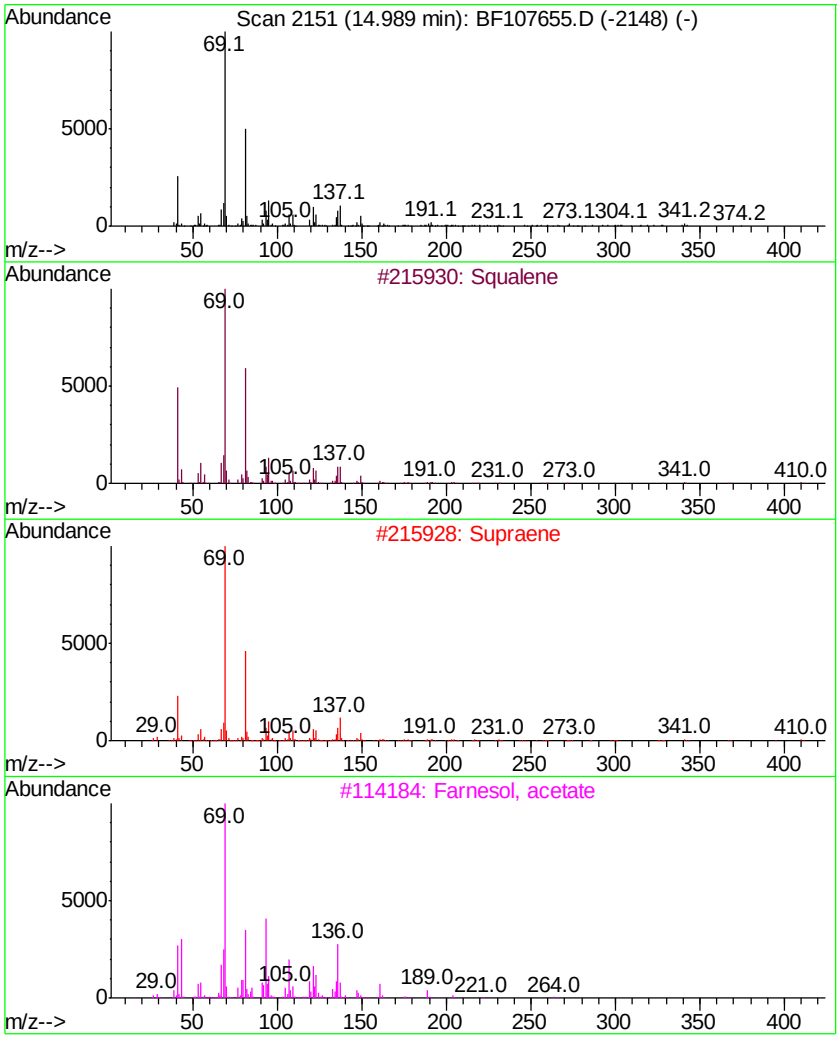
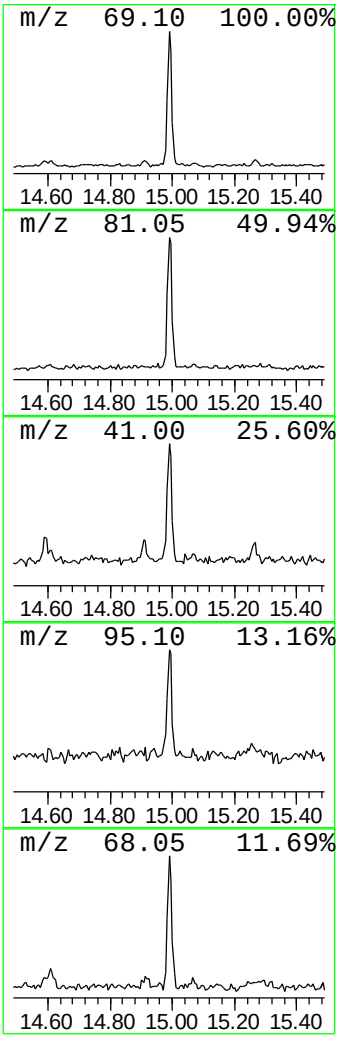
Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	3.71 ng	269249	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	Farnesol, acetate	264	C17H28O2	1000352-67-2	64
4	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	50
5	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	50





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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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...	5.21	11.1	ng	842399	1	6.97	1516830	20.0
unknown6.74	6.74	70.6	ng	5356610	1	6.97	1516830	20.0
n-Hexadecanoic acid	12.01	2.7	ng	275109	4	11.50	2027290	20.0
1-Dodecanol, 2-he...	13.97	3.8	ng	308379	5	14.15	1622430	20.0
Squalene	14.99	3.7	ng	269249	6	15.68	1451240	20.0