LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106654.D
Acq On : 21 Jun 2018 11:52
Operator : JU/SJ
Sample : J3575-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11-D

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-BF061918.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	5.190	482	485	494	rVB	113470	140601	5.80%	0.739%
2	5.601	551	555	559	rBV	1732409	1512840	62.38%	7.950%
3	6.601	721	725	733	rBV	1599281	1630721	67.24%	8.569%
4	6.737	744	748	751	rBV	1826676	1607566	66.28%	8.447%
5	6.960	782	786	789	rVB	615650	512676	21.14%	2.694%
6	7.113	808	812	816	rVB	1375635	1218034	50.22%	6.400%
7	7.525	877	882	889	rBV	1115516	1089760	44.93%	5.726%
8	8.242	1000	1004	1007	rBV	821024	684340	28.22%	3.596%
9	9.313	1182	1186	1190	rBV	1979954	1913444	78.90%	10.055%
10	9.384	1194	1198	1201	rBV2	28841	25686	1.06%	0.135%
11	9.707	1247	1253	1260	rBV	346135	287974	11.87%	1.513%
12	9.913	1284	1288	1292	rBV2	58209	55163	2.27%	0.290%
13	10.001	1299	1303	1307	rVB	1035382	863047	35.59%	4.535%
14	10.413	1370	1373	1376	rVB	74361	56057	2.31%	0.295%
15	10.631	1403	1410	1413	rBV	25035	31478	1.30%	0.165%
16	10.713	1421	1424	1429	rBV	36371	28655	1.18%	0.151%
17	10.795	1434	1438	1441	rBV	1694022	1579191	65.11%	8.298%
18	10.883	1450	1453	1463	rVB	66423	77801	3.21%	0.409%
19	11.336	1526	1530	1532	rBV	37750	31814	1.31%	0.167%
20	11.495	1553	1557	1560	rBV	1125661	990428	40.84%	5.204%
21	13.077	1822	1826	1830	rBV	2372279	2425255	100.00%	12.744%
22	13.630	1916	1920	1923	rBV2	37318	37841	1.56%	0.199%
23	13.960	1973	1976	1986	rBV2	89358	92936	3.83%	0.488%
24	14.148	2003	2008	2011	rBV	890240	840360	34.65%	4.416%
25	14.283	2028	2031	2034	rVB	57669	49126	2.03%	0.258%
26	14.601	2082	2085	2090	rVB	67842	65926	2.72%	0.346%
27	14.918	2135	2139	2144	rBV	70909	82054	3.38%	0.431%
28	15.001	2149	2153	2158	rVV	95407	96685	3.99%	0.508%
29	15.277	2196	2200	2208	rVB	63106	83279	3.43%	0.438%
30	15.689	2264	2270	2276	rVB	561595	808817	33.35%	4.250%
31	16.142	2343	2347	2352	rVB2	39455	58114	2.40%	0.305%
32	16.677	2434	2438	2446	rVB4	30530	52953	2.18%	0.278%

LSC Area Percent Report

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Acq On : 21 Jun 2018 11:52
Operator : JU/SJ
Sample : J3575-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-11-D

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-BF061918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 19030622

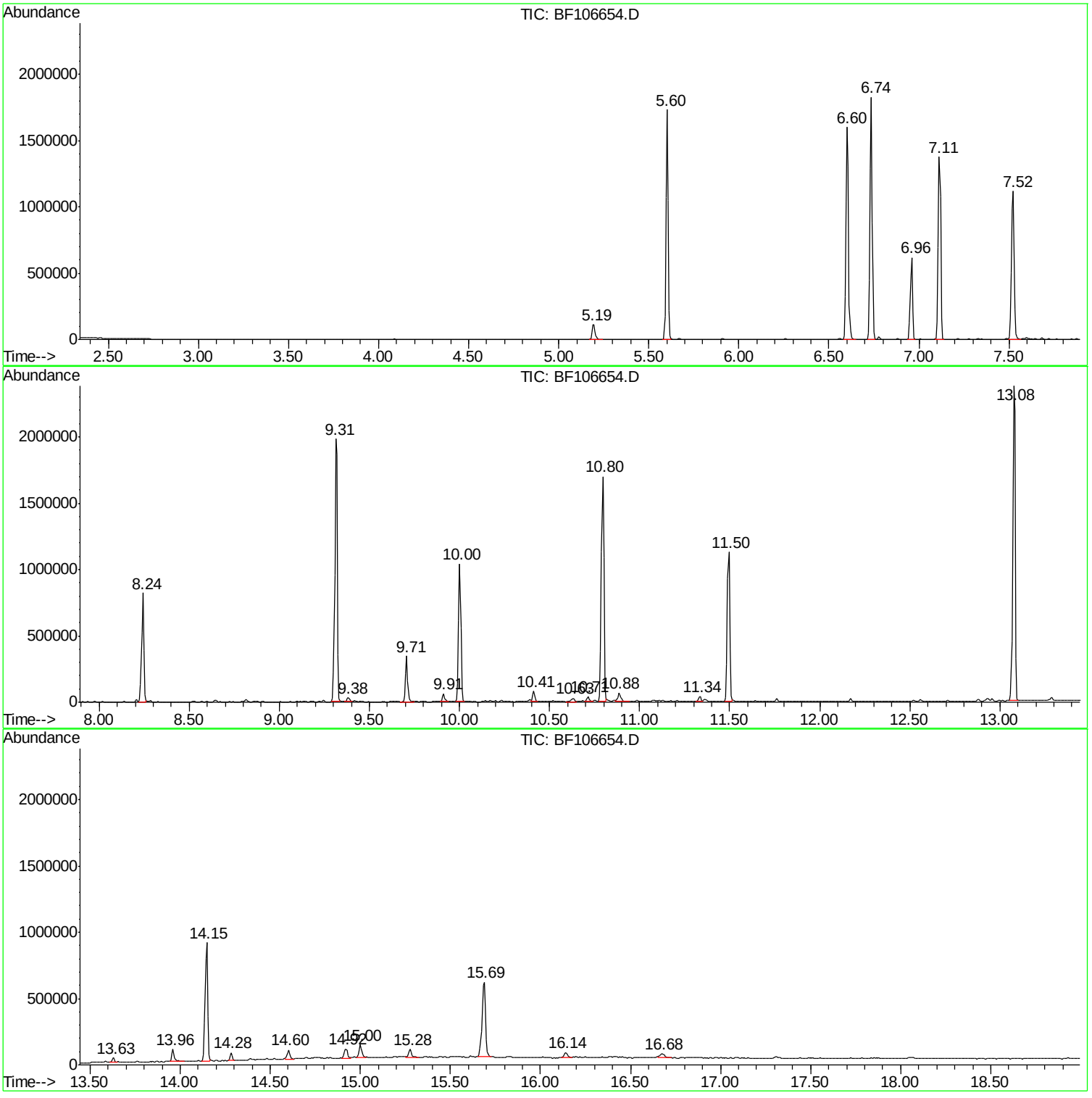
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106654.D
Acq On : 21 Jun 2018 11:52
Operator : JU/SJ
Sample : J3575-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106654.D
Acq On : 21 Jun 2018 11:52
Operator : JU/SJ
Sample : J3575-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

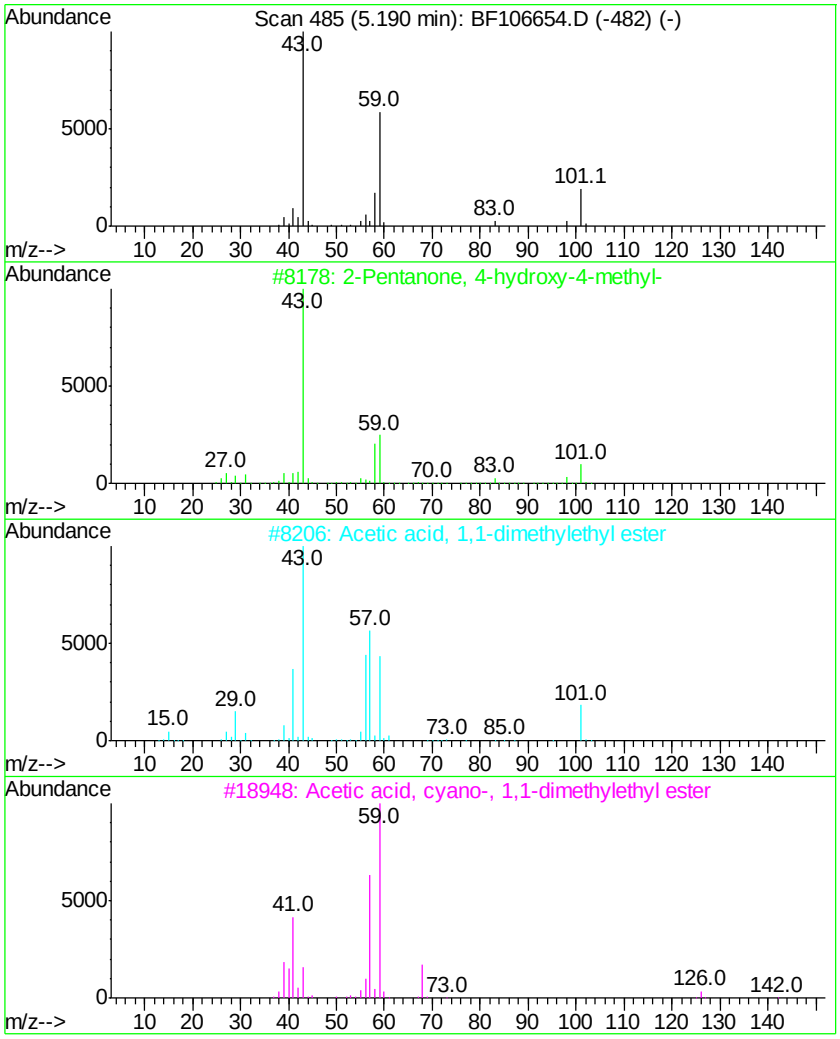
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

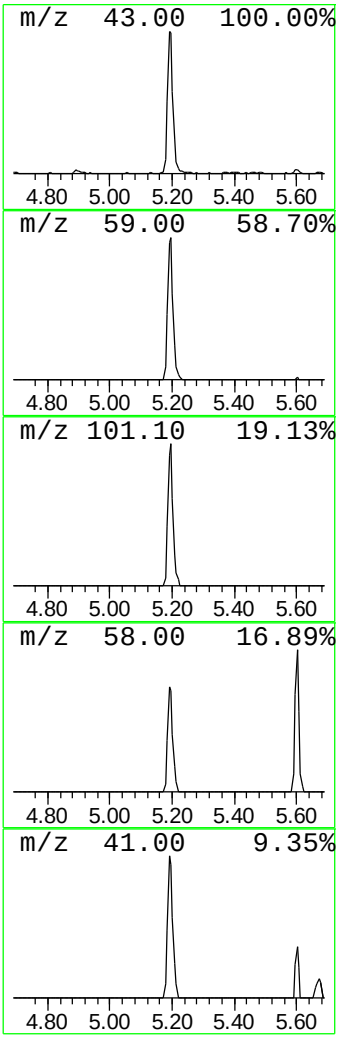
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	5.48 ng	140601	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106654.D
Acq On : 21 Jun 2018 11:52
Operator : JU/SJ
Sample : J3575-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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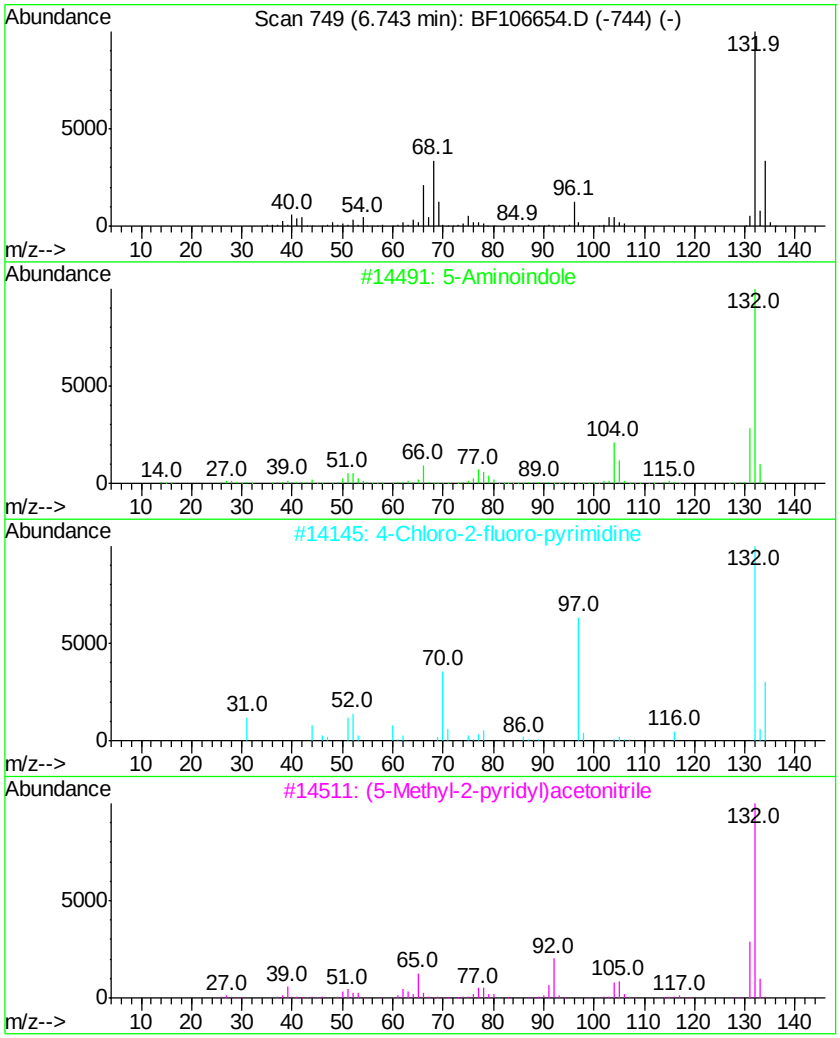
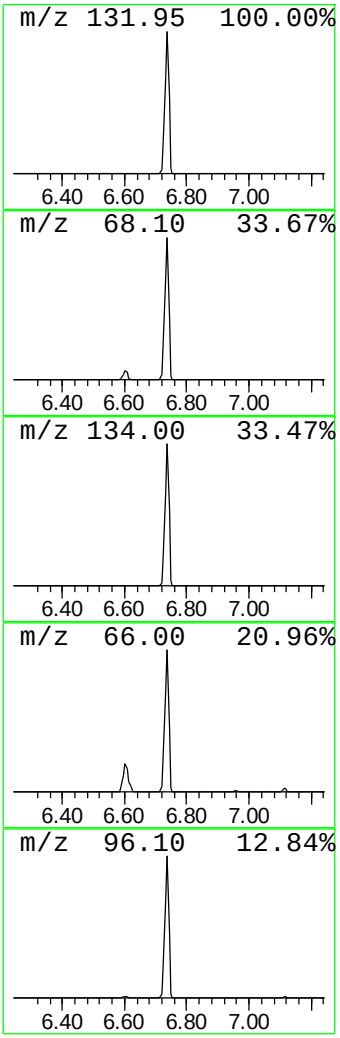
Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	62.71 ng	1607570	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106654.D
Acq On : 21 Jun 2018 11:52
Operator : JU/SJ
Sample : J3575-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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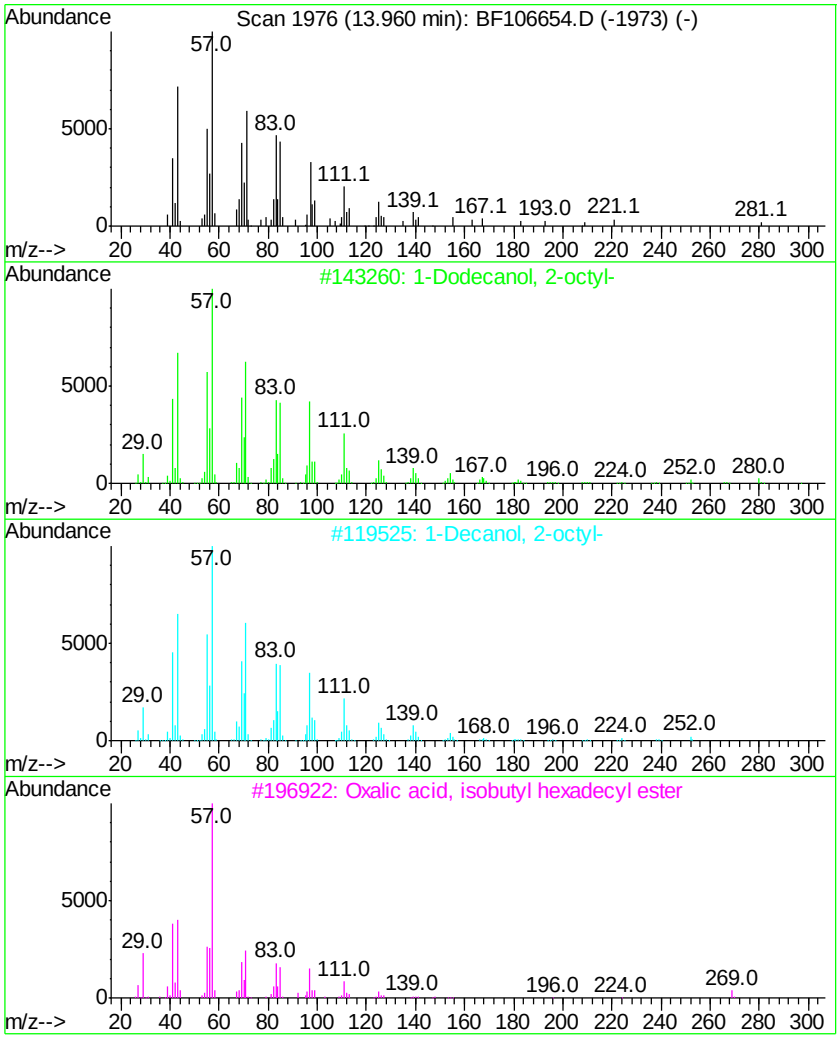
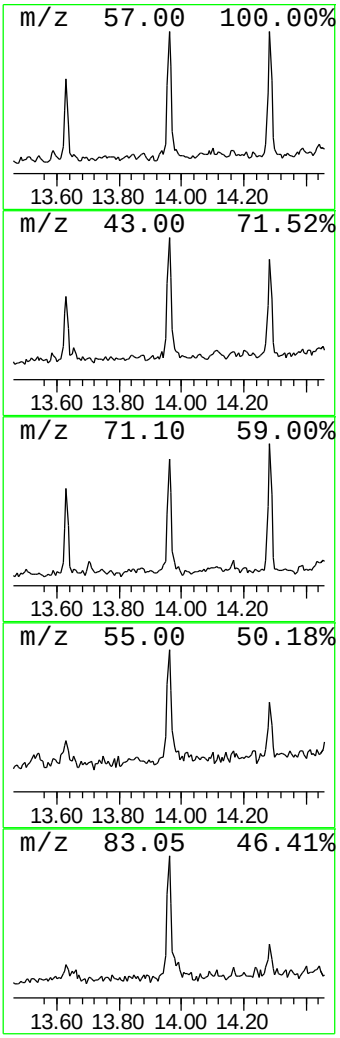
Peak Number 4 1-Dodecanol, 2-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	2.21 ng	92936	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
2	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	91
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	87
5	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106654.D
Acq On : 21 Jun 2018 11:52
Operator : JU/SJ
Sample : J3575-18
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Instrument : BNA_F
ClientSampleId : TP-11-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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TIC Library : C:\DATABASE\NIST11.L
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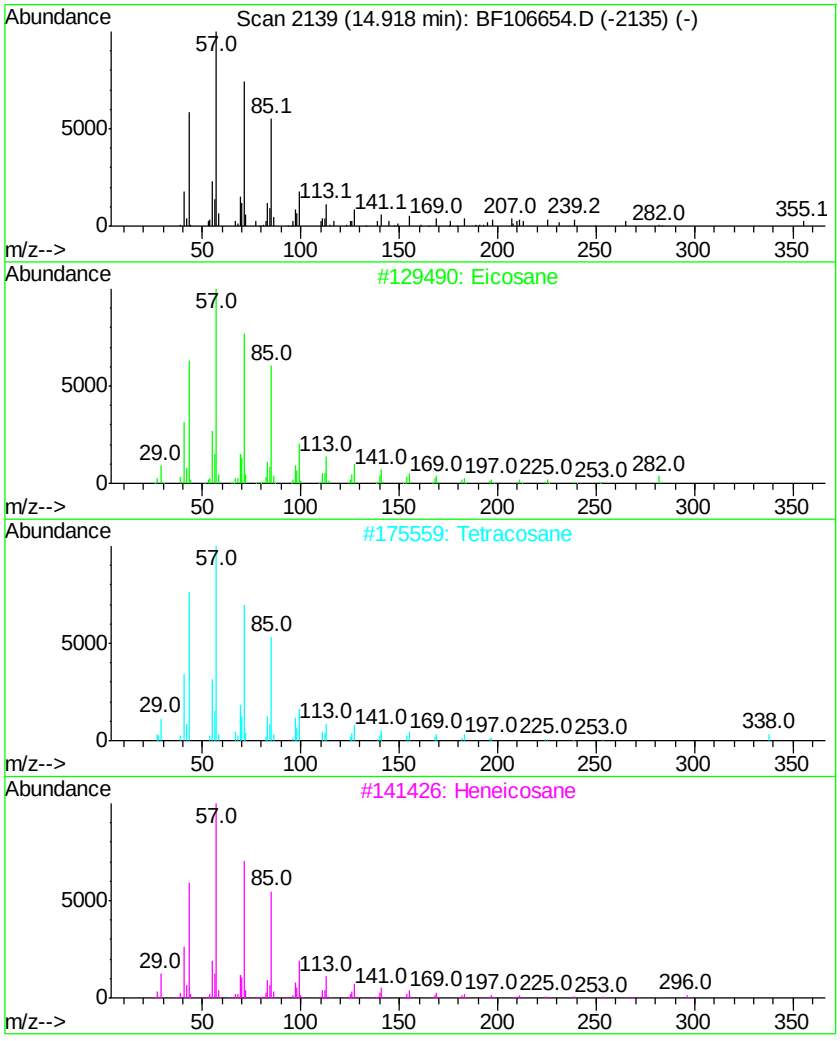
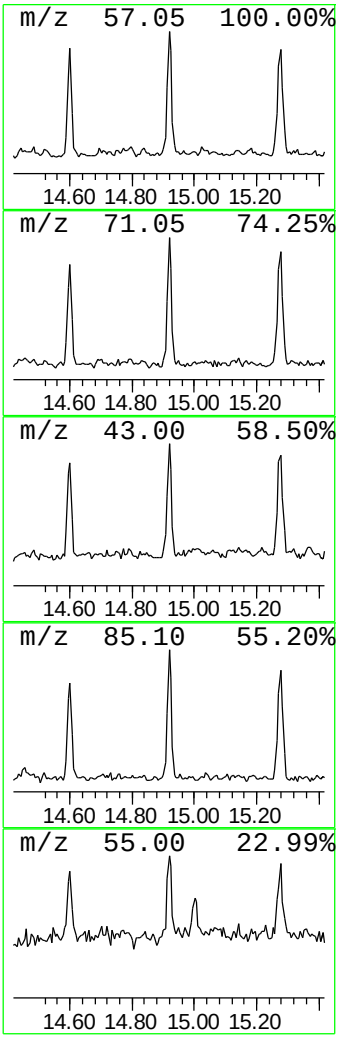
Peak Number 5 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	2.03 ng	82054	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octadecane	254	C18H38	000593-45-3	91
5	Hexacosane	366	C26H54	000630-01-3	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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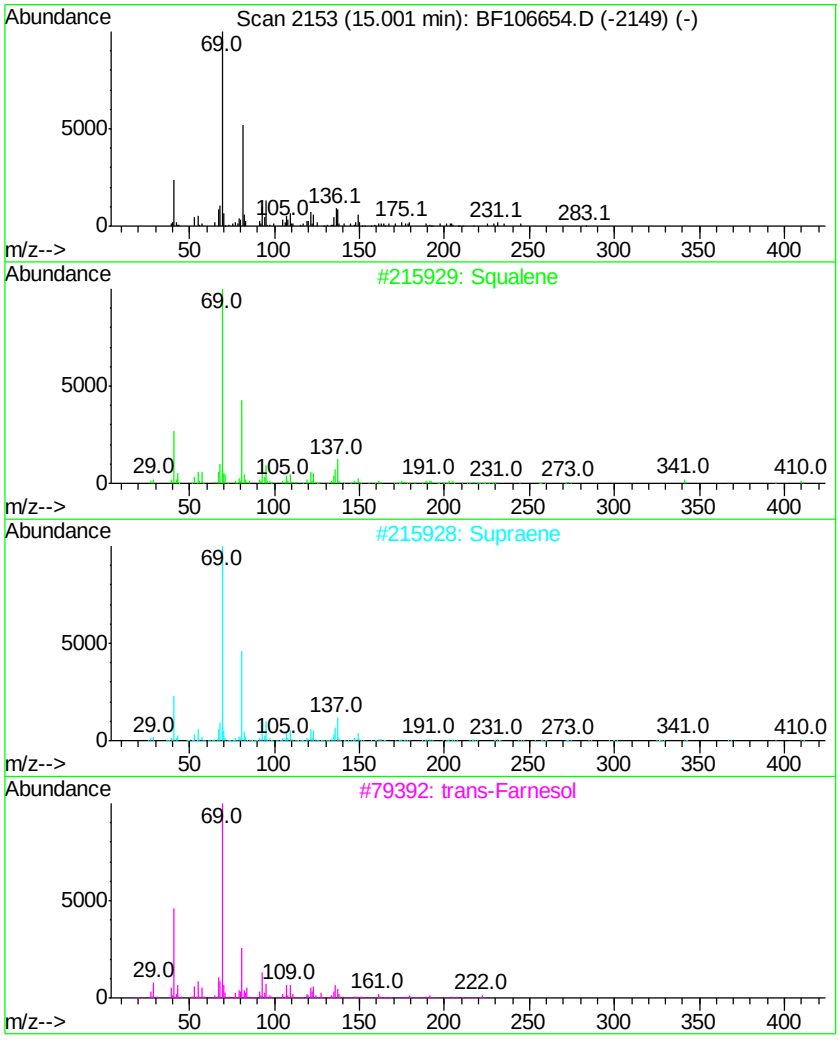
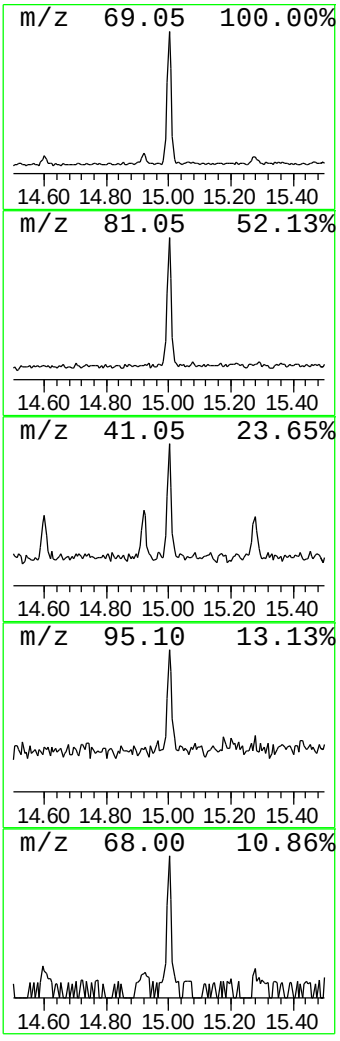
Peak Number 6 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	2.39 ng	96685	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Supraene	410	C30H50	007683-64-9	87
3	trans-Farnesol	222	C15H26O	000106-28-5	72
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





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Sample : J3575-18
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-11-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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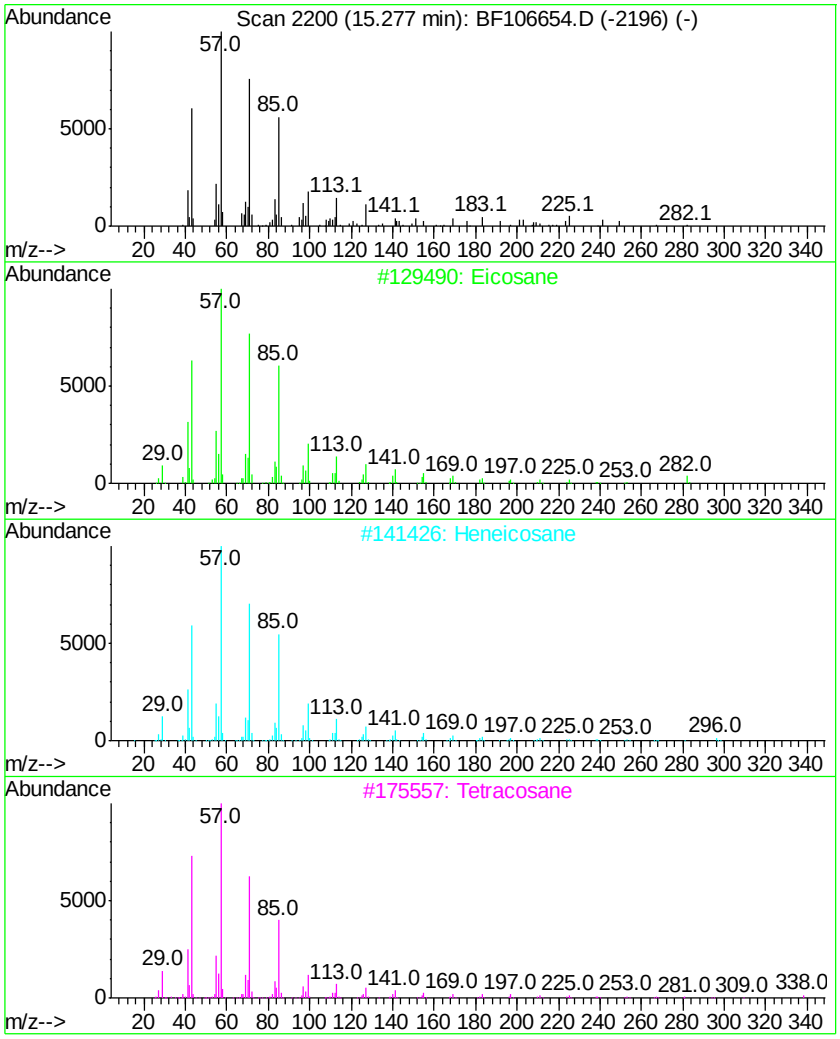
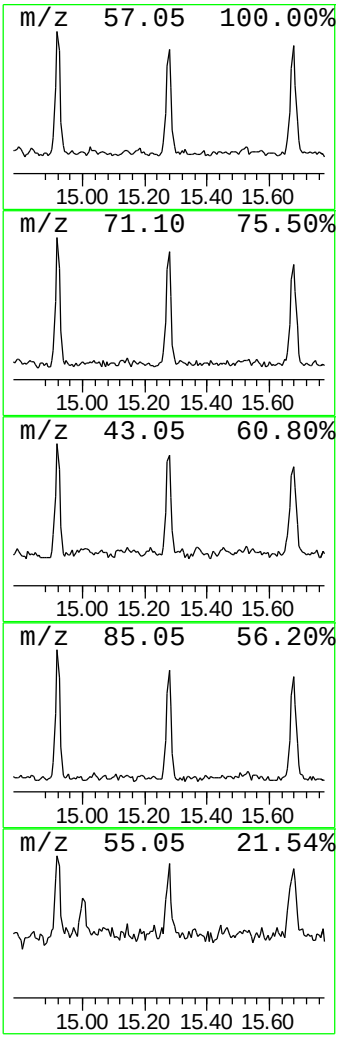
Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	2.06 ng	83279	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	90
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	90
5	Pentacosane	352	C25H52	000629-99-2	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062118\
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Instrument : BNA_F
ClientSampleId : TP-11-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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
2-Pentanone, 4-hy...	5.19	5.5	ng	140601	1	6.96	512676	20.0
unknown6.74	6.74	62.7	ng	1607570	1	6.96	512676	20.0
1-Dodecanol, 2-oc...	13.96	2.2	ng	92936	5	14.15	840360	20.0
Tetracosane	14.92	2.0	ng	82054	6	15.69	808817	20.0
Squalene	15.00	2.4	ng	96685	6	15.69	808817	20.0
Eicosane	15.28	2.1	ng	83279	6	15.69	808817	20.0