LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108731.D
Acq On : 1 Sep 2018 11:00
Operator : JU/SJ
Sample : J4729-17
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-TIPC-E-U-B

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-BF083018.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	5.707	562	573	574	rBV5	16062	39170	1.70%	0.341%
2	6.666	731	736	740	rBV2	29084	62827	2.73%	0.547%
3	6.778	751	755	775	rBV	231970	687117	29.85%	5.981%
4	7.007	790	794	811	rBV	96443	291360	12.66%	2.536%
5	7.154	815	819	852	rVB	867406	1435273	62.35%	12.493%
6	7.572	886	890	910	rBV	259554	894652	38.87%	7.787%
7	8.283	1007	1011	1037	rBV	124333	382655	16.62%	3.331%
8	9.354	1189	1193	1229	rBV	1223492	2043031	88.76%	17.783%
9	9.742	1256	1259	1269	rBV	78275	120671	5.24%	1.050%
10	10.042	1306	1310	1329	rBV	291556	446560	19.40%	3.887%
11	10.695	1418	1421	1428	rBV	75039	71941	3.13%	0.626%
12	10.836	1441	1445	1470	rBV	348877	792979	34.45%	6.902%
13	11.542	1561	1565	1585	rBV	273650	543331	23.60%	4.729%
14	13.118	1829	1833	1856	rBV	1916176	2301862	100.00%	20.036%
15	14.083	1990	1997	2000	rBV4	30945	69814	3.03%	0.608%
16	14.195	2012	2016	2025	rBV	400946	570344	24.78%	4.964%
17	14.259	2025	2027	2032	rVV3	20713	24648	1.07%	0.215%
18	14.307	2032	2035	2039	rVB	25685	23509	1.02%	0.205%
19	14.612	2084	2087	2092	rBB2	31774	30343	1.32%	0.264%
20	14.936	2139	2142	2146	rBV	40071	40184	1.75%	0.350%
21	15.018	2153	2156	2163	rVB	62642	69344	3.01%	0.604%
22	15.295	2200	2203	2208	rBV	42540	50901	2.21%	0.443%
23	15.706	2268	2273	2276	rBV	40841	53070	2.31%	0.462%
24	15.753	2276	2281	2293	rVV	184288	363678	15.80%	3.166%
25	16.171	2347	2352	2361	rBV	33104	52978	2.30%	0.461%
26	16.718	2441	2445	2450	rVB3	16873	26368	1.15%	0.230%

Sum of corrected areas: 11488610

LSC Report - Integrated Chromatogram

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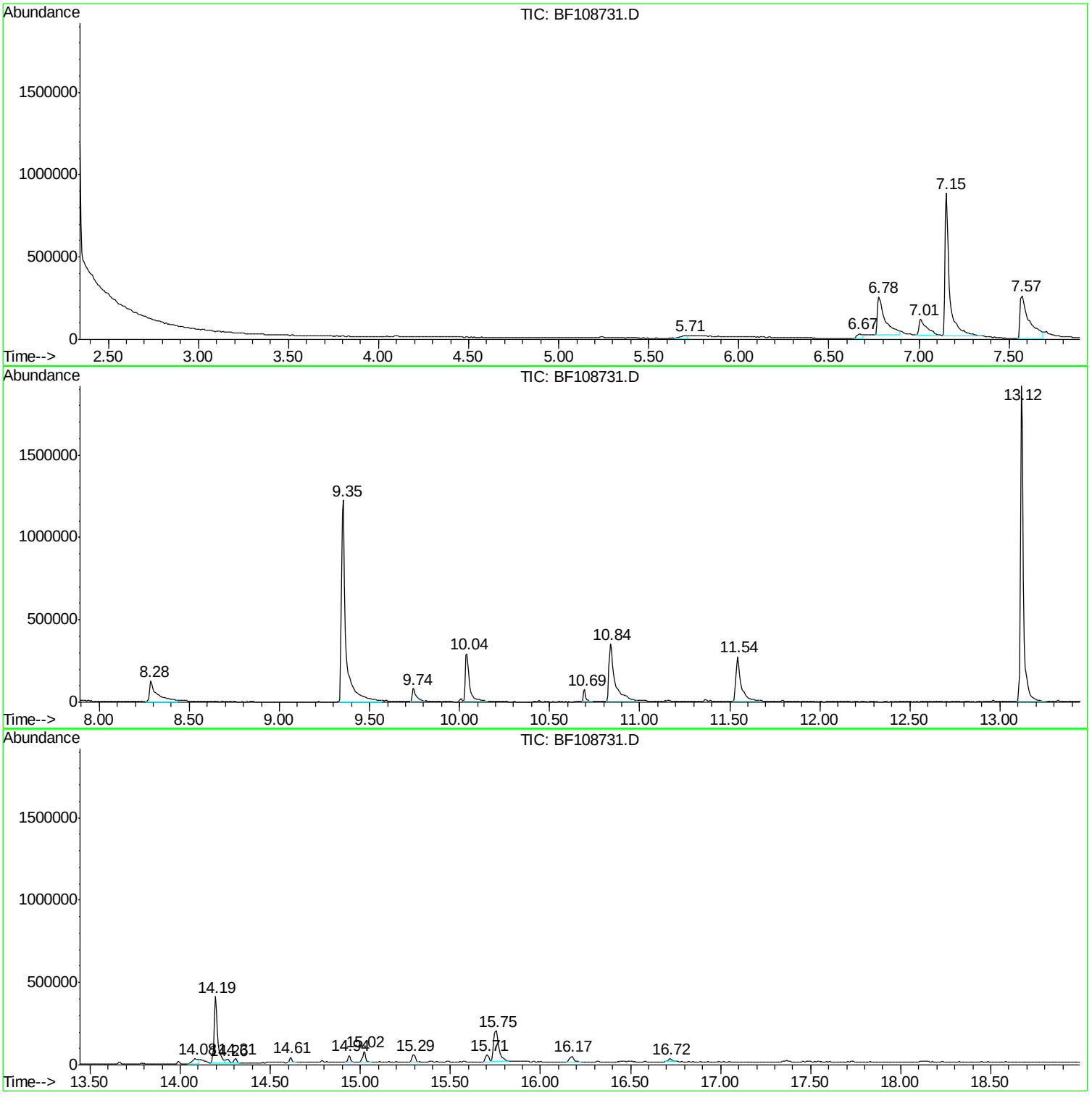
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-TIPC-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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\BF083118\
Data File : BF108731.D
Acq On : 1 Sep 2018 11:00
Operator : JU/SJ
Sample : J4729-17
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-TIPC-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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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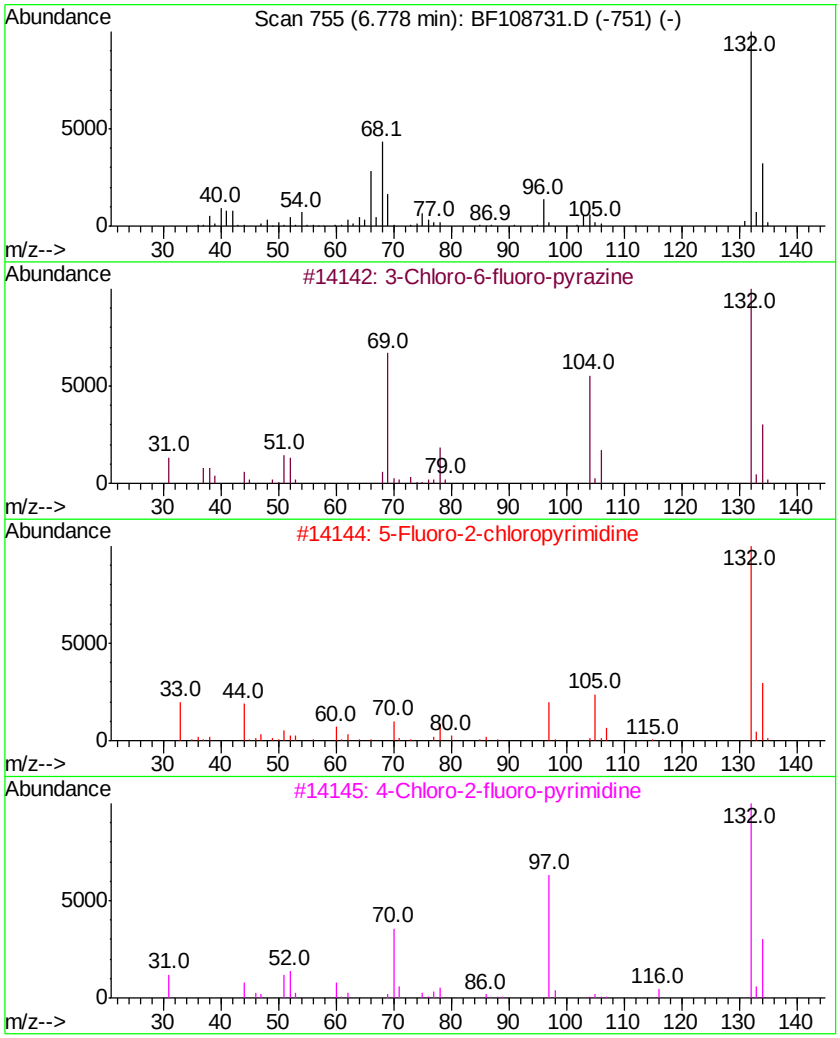
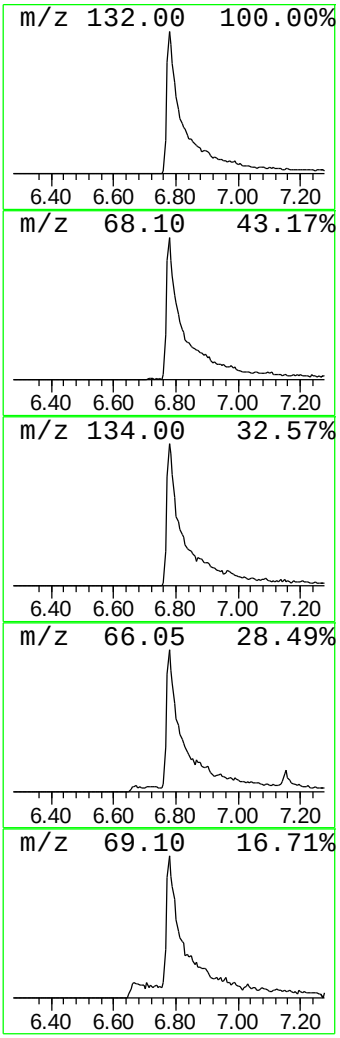
Peak Number 1 unknown6.78 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	47.17 ng	687117	1,4-Dichlorobenzene-d4	7.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	12
4	Xenon	132	Xe	007440-63-3	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





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Data File : BF108731.D
Acq On : 1 Sep 2018 11:00
Operator : JU/SJ
Sample : J4729-17
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-TIPC-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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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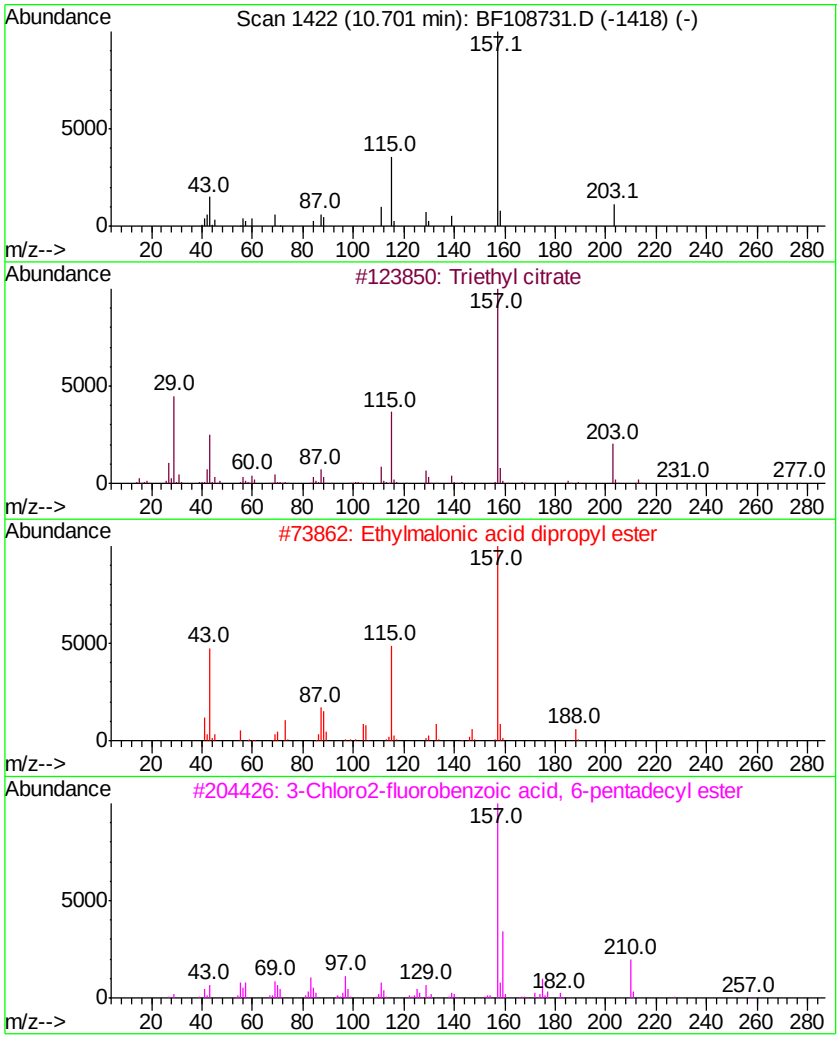
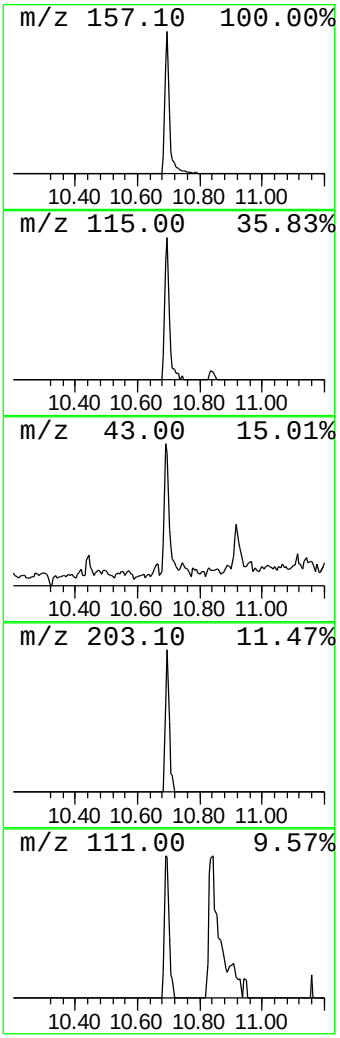
Peak Number 3 Triethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	3.22 ng	71941	Acenaphthene-d10	10.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	86
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3	3-Chloro2-fluorobenzoic acid, 6-...	384	C22H34ClFO2	1000338-65-3	40
4	2-Chlorobenzoic acid, hexadecyl ...	380	C23H37ClO2	070152-86-2	38
5	Adipic acid, ethyl pent-4-en-2-y...	242	C13H22O4	1000354-11-7	33





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108731.D
Acq On : 1 Sep 2018 11:00
Operator : JU/SJ
Sample : J4729-17
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-TIPC-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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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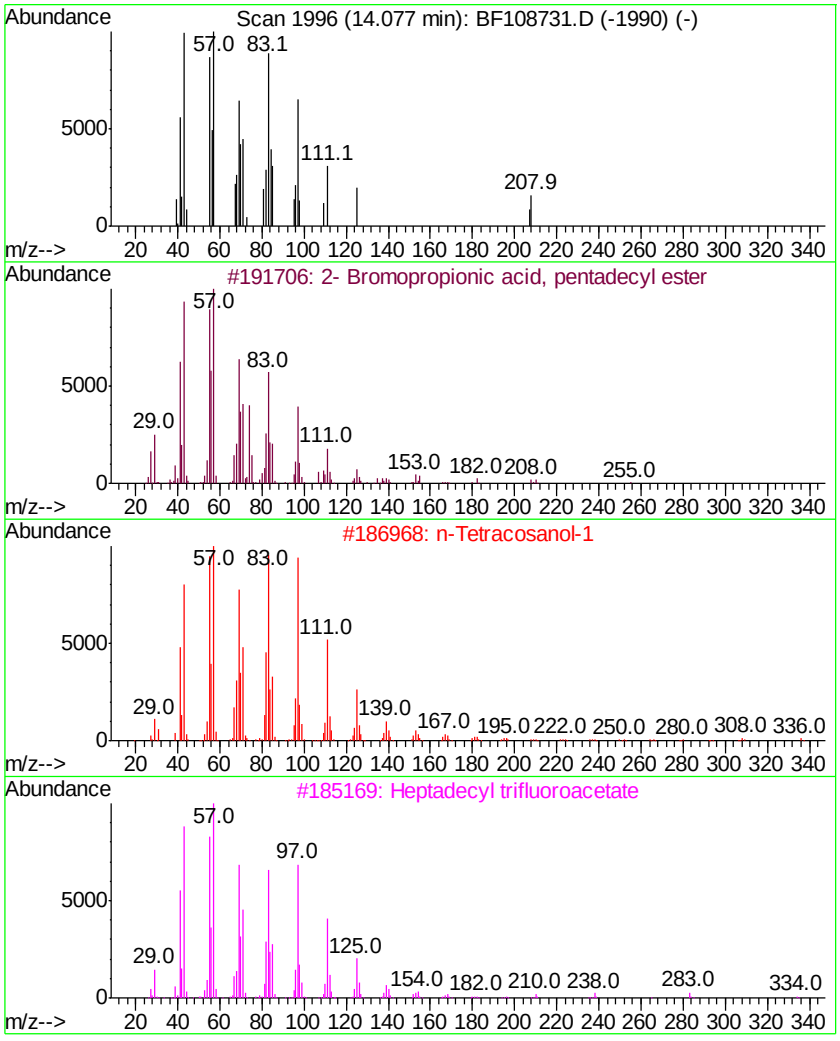
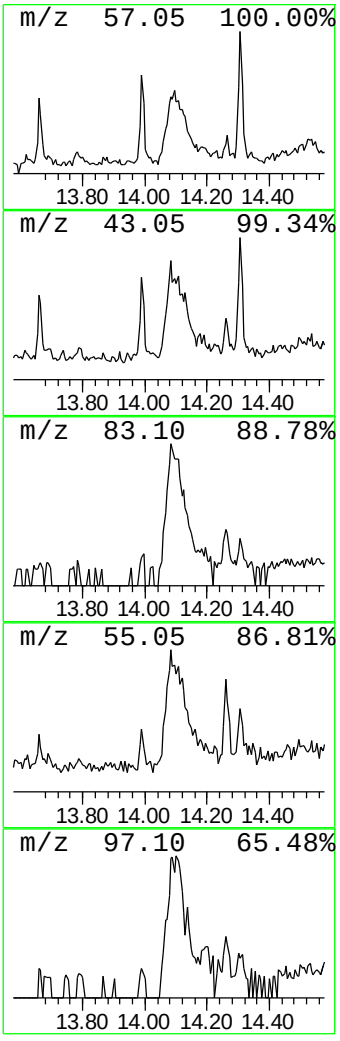
Peak Number 4 2- Bromopropionic acid, pen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.08	2.45 ng	69814	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	90
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	86
4	Behenic alcohol	326	C22H46O	000661-19-8	83
5	1-Heptacosanol	396	C27H56O	002004-39-9	83





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Data File : BF108731.D
Acq On : 1 Sep 2018 11:00
Operator : JU/SJ
Sample : J4729-17
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-TIPC-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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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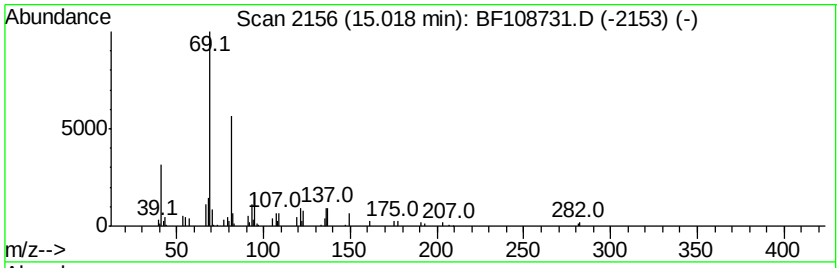
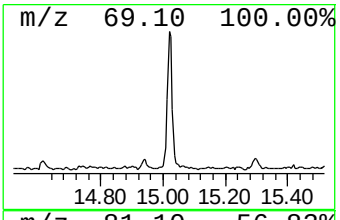
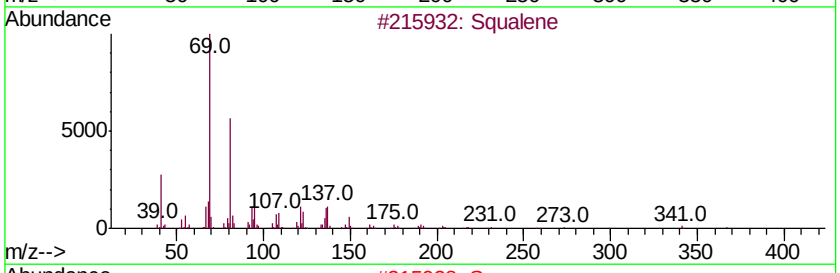
Peak Number 5 Squalene Concentration Rank 3

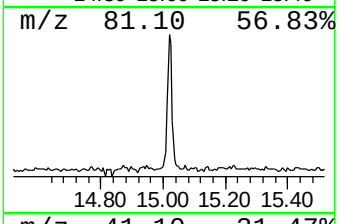
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	3.81 ng	69344	Perylene-d12	15.75

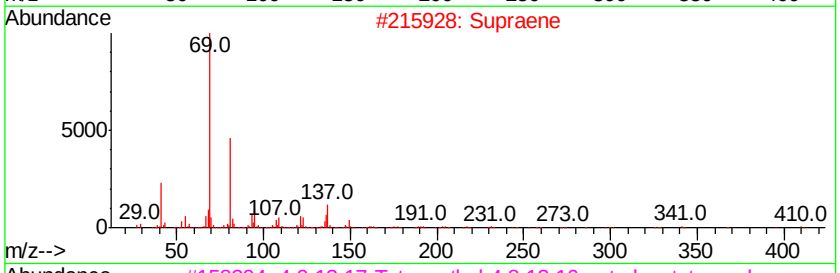
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	90
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5	trans-Farnesol	222	C15H26O	000106-28-5	72

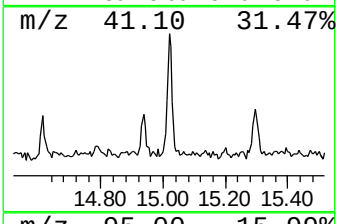


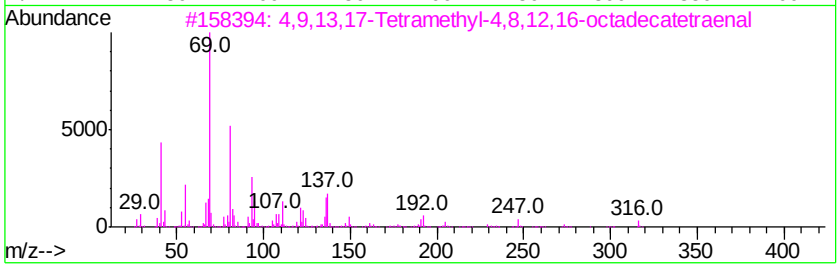


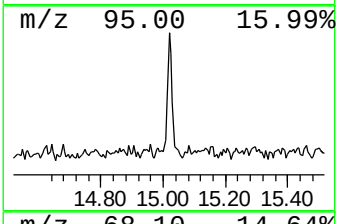


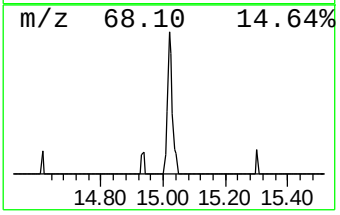












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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

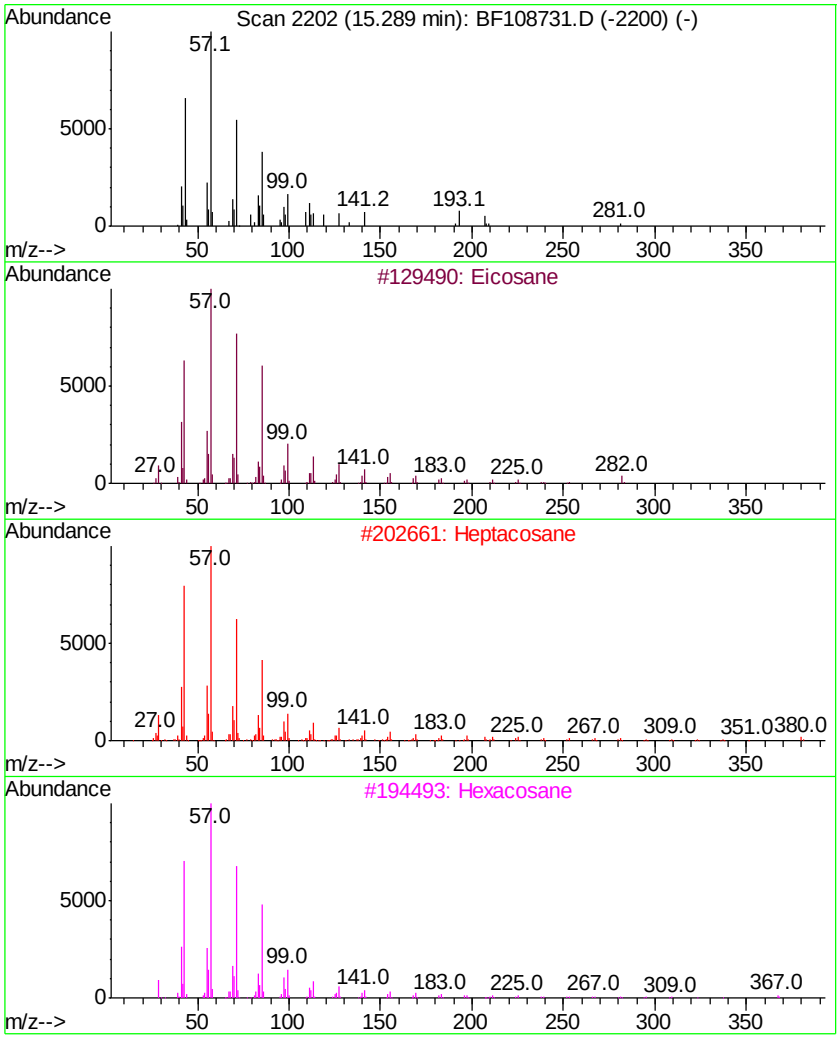
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

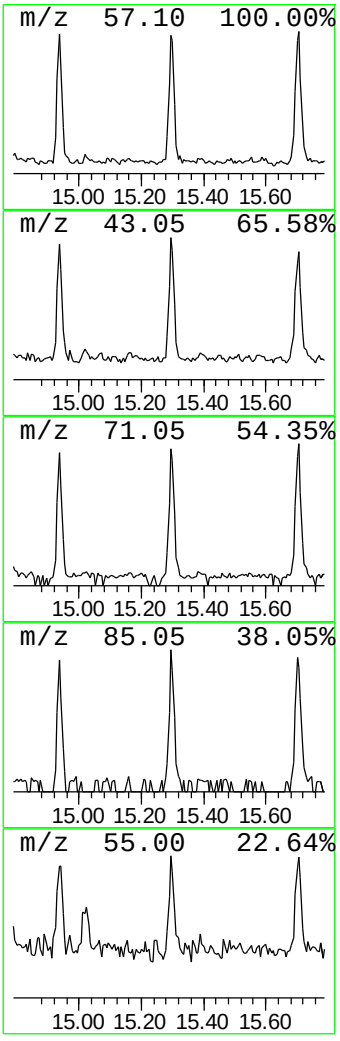
****

Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	2.80 ng	50901	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heptacosane	380	C27H56	000593-49-7	90
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Octacosane	394	C28H58	000630-02-4	83





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TIC Library : C:\DATABASE\NIST11.L
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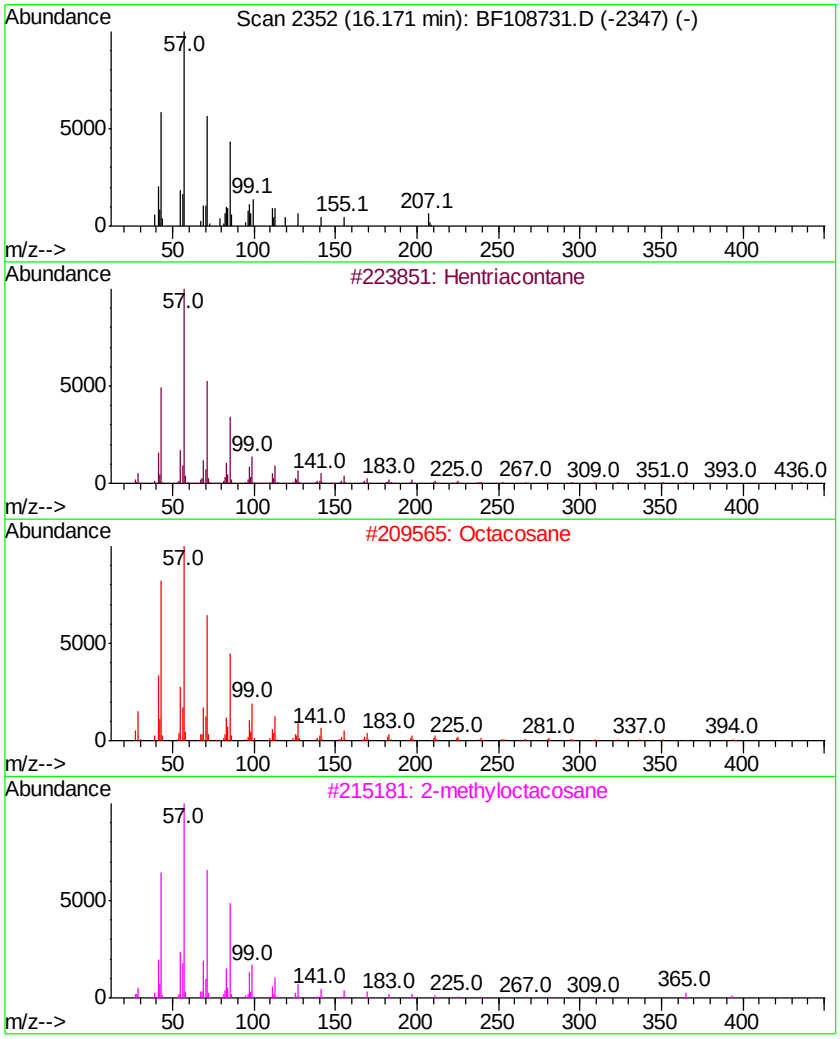
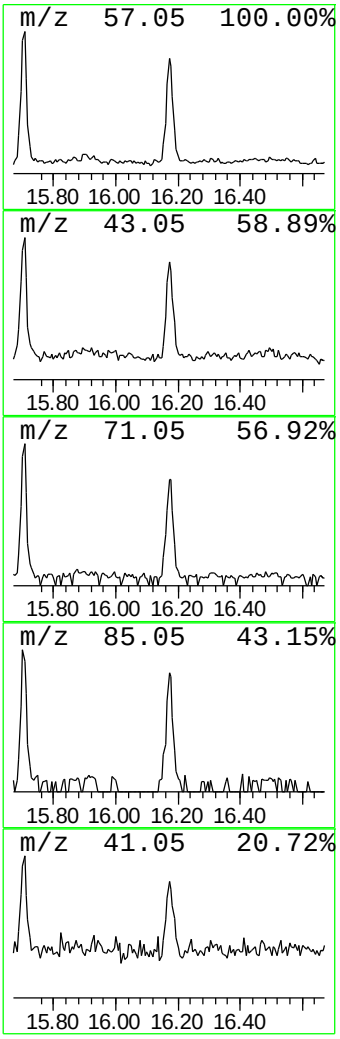
Peak Number 7 Hentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	2.91 ng	52978	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Octacosane	394	C28H58	000630-02-4	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heneicosane	296	C21H44	000629-94-7	87





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.78	6.78	47.2	ng	687117	1	7.01	291360	20.0
Triethyl citrate	10.70	3.2	ng	71941	3	10.04	446560	20.0
2- Bromopropionic...	14.08	2.5	ng	69814	5	14.19	570344	20.0
Squalene	15.02	3.8	ng	69344	6	15.75	363678	20.0
Eicosane	15.29	2.8	ng	50901	6	15.75	363678	20.0
Hentriacontane	16.17	2.9	ng	52978	6	15.75	363678	20.0