LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107567.D
Acq On : 21 Jul 2018 11:10
Operator : JU/SJ
Sample : J4061-10
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071718-TIPC-F-U-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	5.201	484	487	496	rBV	164639	184640	2.37%	0.361%
2	5.601	551	555	579	rBV	1956033	2758749	35.34%	5.399%
3	6.601	721	725	745	rBV	1202940	2021254	25.90%	3.956%
4	6.742	745	749	773	rVB	4316400	4749904	60.85%	9.295%
5	6.972	785	788	810	rVB	1563120	1832517	23.48%	3.586%
6	7.131	810	815	836	rBV	6036470	6332112	81.12%	12.392%
7	7.537	879	884	894	rBV	4185242	5038347	64.55%	9.860%
8	8.254	1002	1006	1023	rBV	1946705	2132968	27.33%	4.174%
9	9.331	1184	1189	1204	rBV	7478798	7805509	100.00%	15.275%
10	9.725	1252	1256	1262	rBV	108661	117650	1.51%	0.230%
11	10.013	1302	1305	1322	rVB	1745183	1846843	23.66%	3.614%
12	10.678	1415	1418	1426	rBV	384452	300158	3.85%	0.587%
13	10.807	1436	1440	1454	rBV	2718067	2859112	36.63%	5.595%
14	11.507	1556	1559	1575	rVB	1580860	1699103	21.77%	3.325%
15	12.019	1642	1646	1655	rBV2	96636	136261	1.75%	0.267%
16	13.095	1825	1829	1845	rVB	6096194	6256088	80.15%	12.243%
17	13.977	1976	1979	1986	rBV	95119	115592	1.48%	0.226%
18	14.160	2006	2010	2022	rBV	2067463	1959111	25.10%	3.834%
19	14.607	2082	2086	2089	rBV2	125450	136033	1.74%	0.266%
20	14.924	2137	2140	2143	rVB	180930	168921	2.16%	0.331%
21	15.283	2197	2201	2205	rBV	221119	248999	3.19%	0.487%
22	15.695	2265	2271	2278	rBV3	1232973	1846491	23.66%	3.614%
23	16.154	2344	2349	2354	rVB	171653	260300	3.33%	0.509%
24	16.695	2435	2441	2446	rBV2	108565	201646	2.58%	0.395%
25	17.336	2545	2550	2557	rVB5	43371	91111	1.17%	0.178%

Sum of corrected areas: 51099419

LSC Report - Integrated Chromatogram

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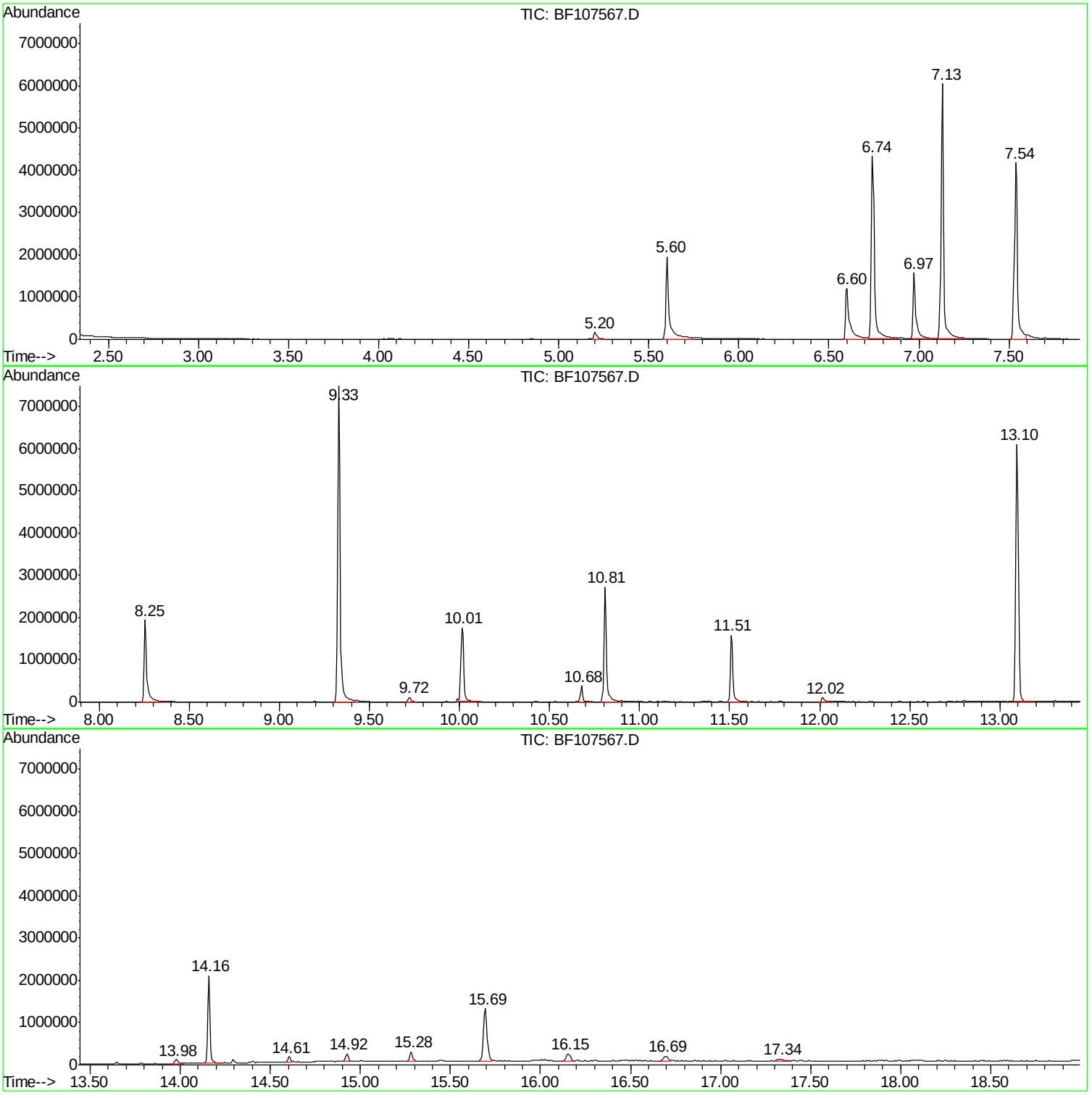
Sample : J4061-10
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071718-TIPC-F-U-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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107567.D
Acq On : 21 Jul 2018 11:10
Operator : JU/SJ
Sample : J4061-10
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071718-TIPC-F-U-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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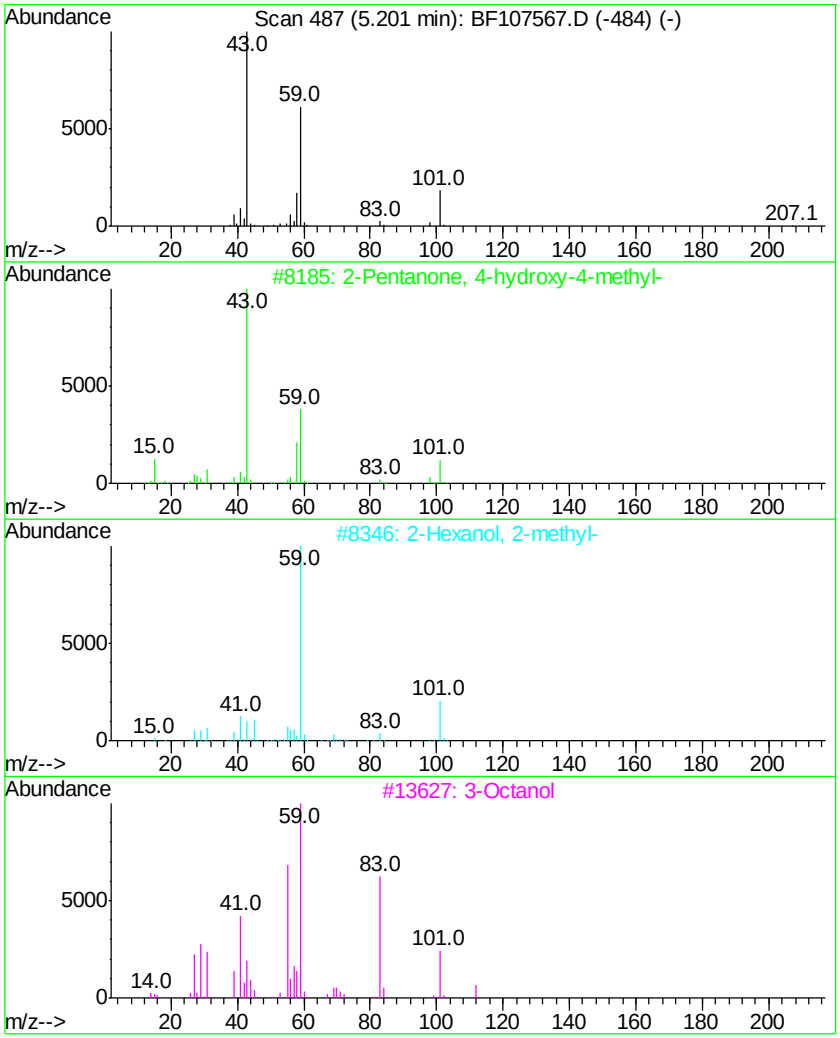
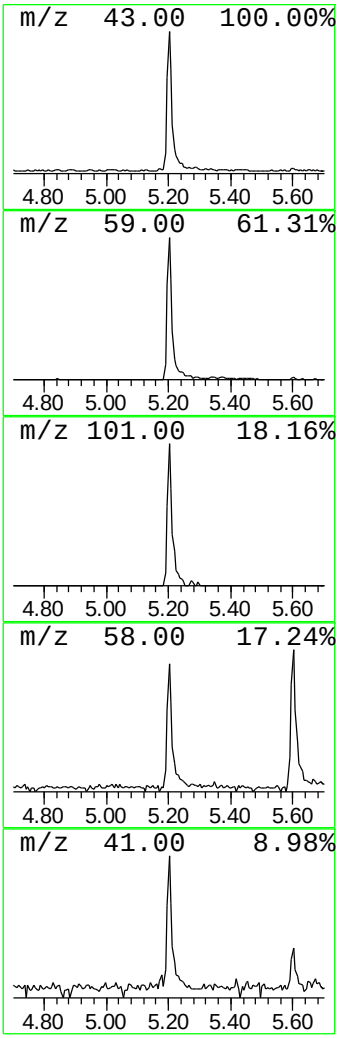
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.02 ng	184640	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	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	3-Octanol	130	C8H18O	000589-98-0	36
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	9





Library Search Compound Report

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Data File : BF107567.D
Acq On : 21 Jul 2018 11:10
Operator : JU/SJ
Sample : J4061-10
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071718-TIPC-F-U-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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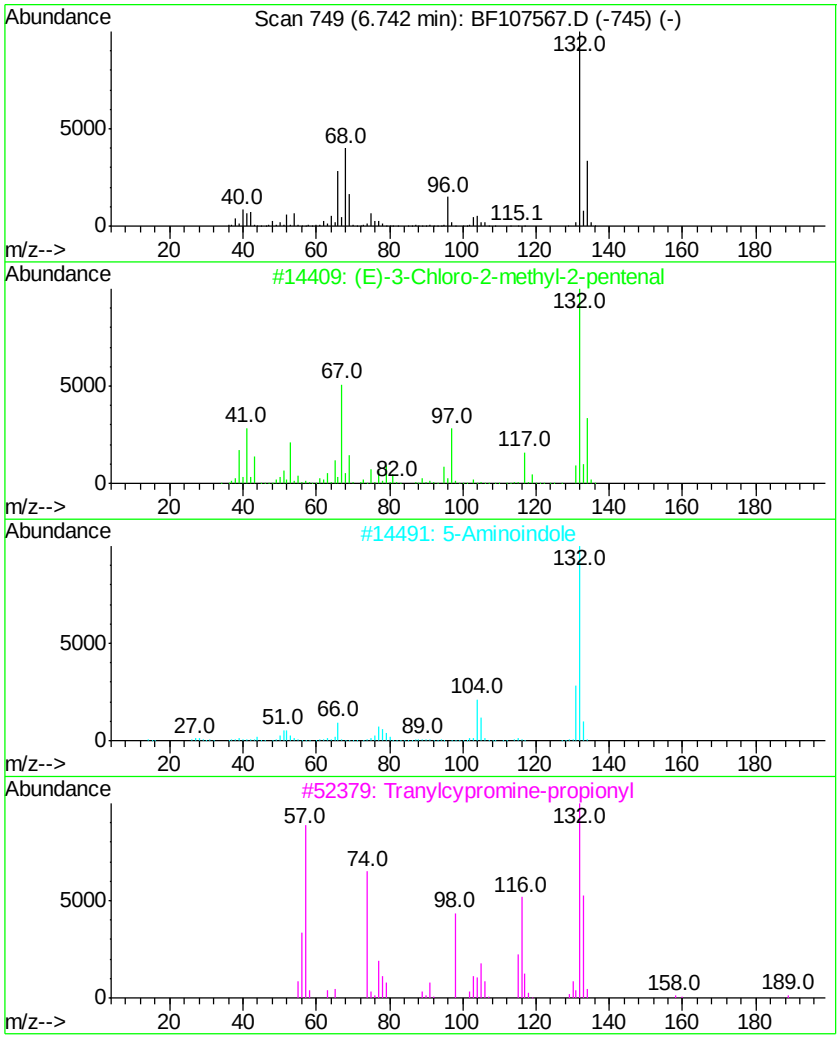
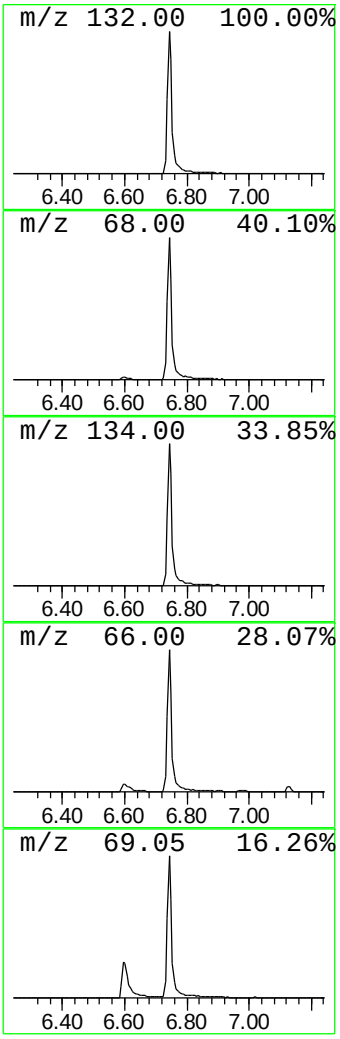
Peak Number 2 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	51.84 ng	4749900	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
Data File : BF107567.D
Acq On : 21 Jul 2018 11:10
Operator : JU/SJ
Sample : J4061-10
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071718-TIPC-F-U-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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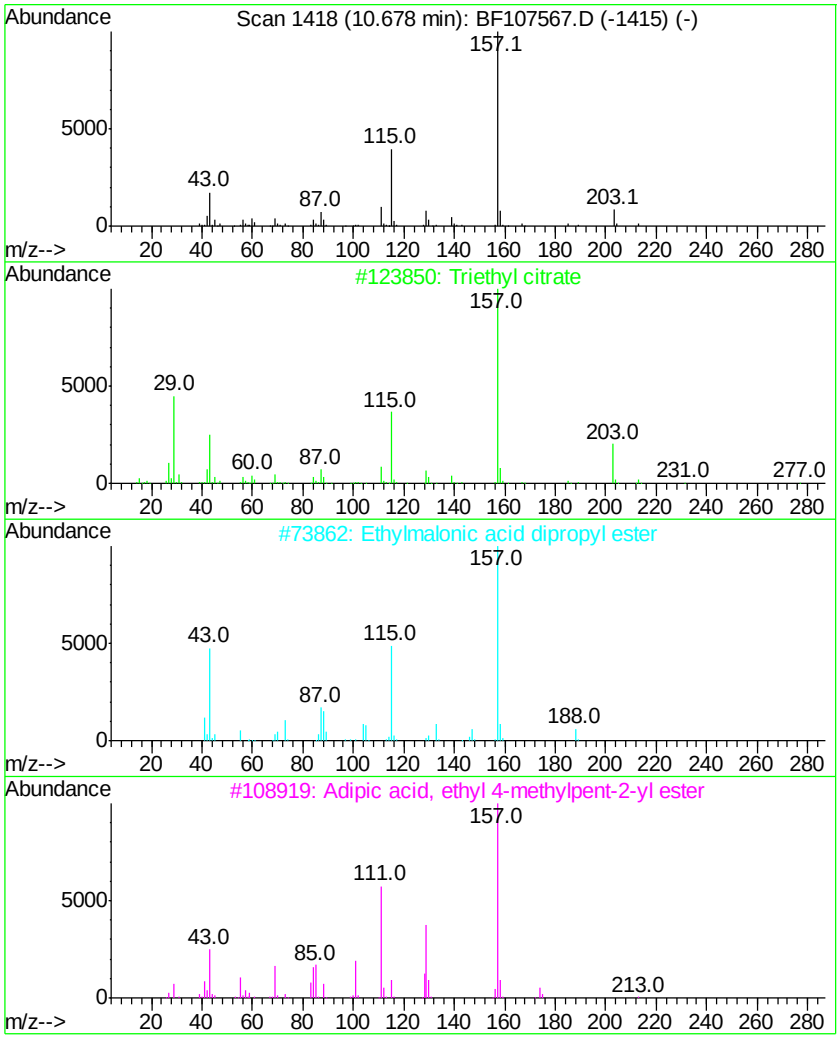
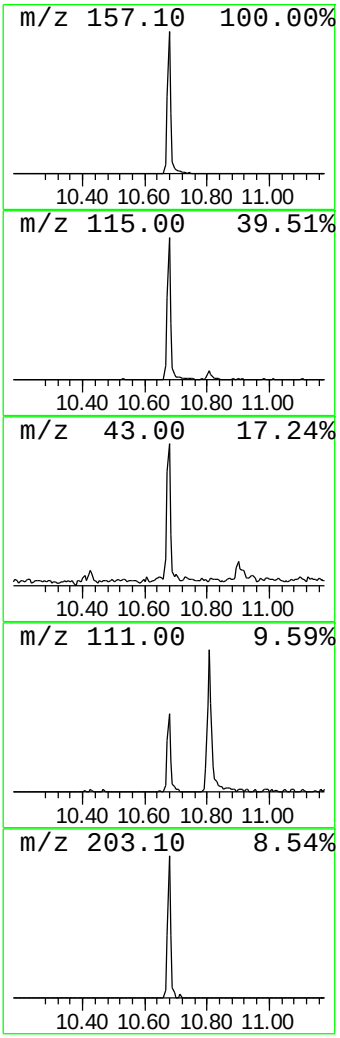
Peak Number 4 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	3.25 ng	300158	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	91
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	45
3	Adipic acid, ethyl 4-methylpent-...	258	C14H26O4	1000353-49-9	38
4	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	37
5	3-Chloro2-fluorobenzoic acid, 4-...	356	C20H30ClFO2	1000338-64-4	33





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
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Acq On : 21 Jul 2018 11:10
Operator : JU/SJ
Sample : J4061-10
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071718-TIPC-F-U-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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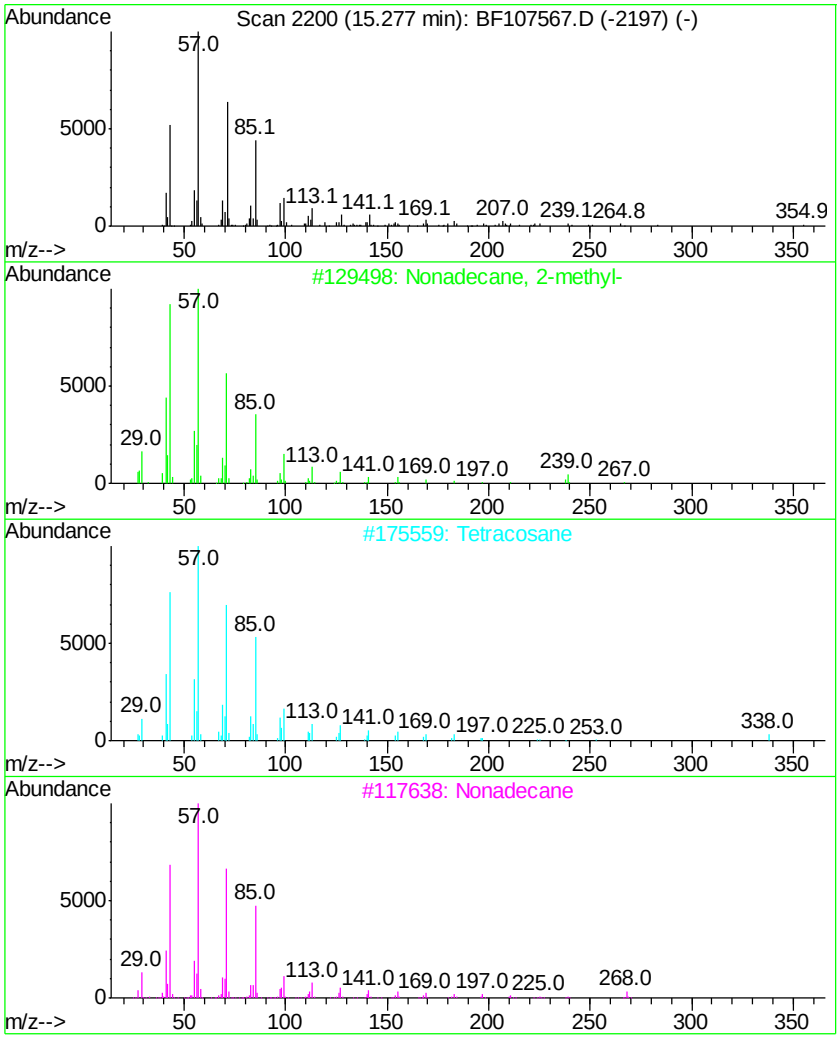
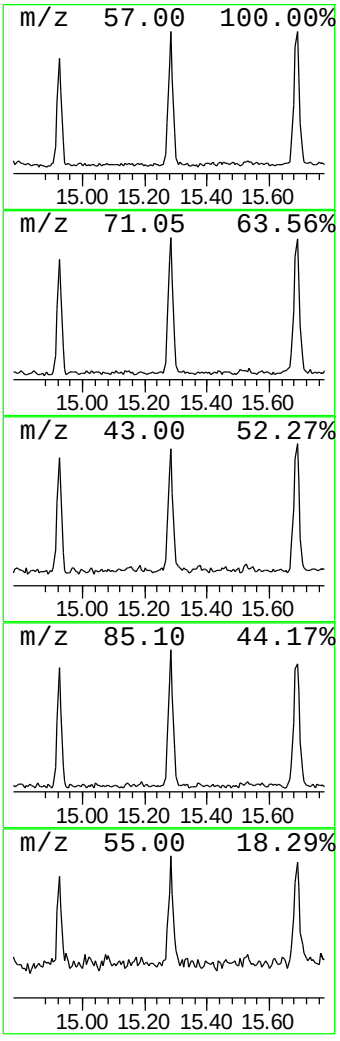
Peak Number 5 Nonadecane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	2.70 ng	248999	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
2	Tetracosane	338	C24H50	000646-31-1	87
3	Nonadecane	268	C19H40	000629-92-5	86
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5	Eicosane	282	C20H42	000112-95-8	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072018\
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Acq On : 21 Jul 2018 11:10
Operator : JU/SJ
Sample : J4061-10
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071718-TIPC-F-U-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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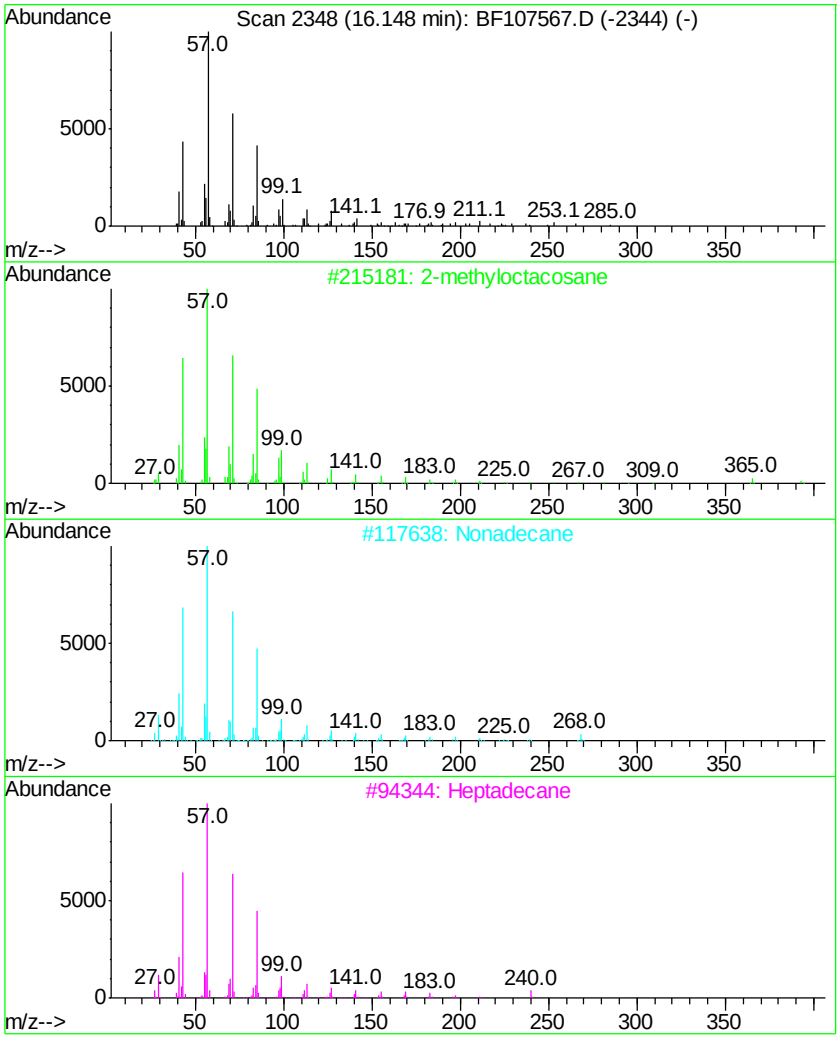
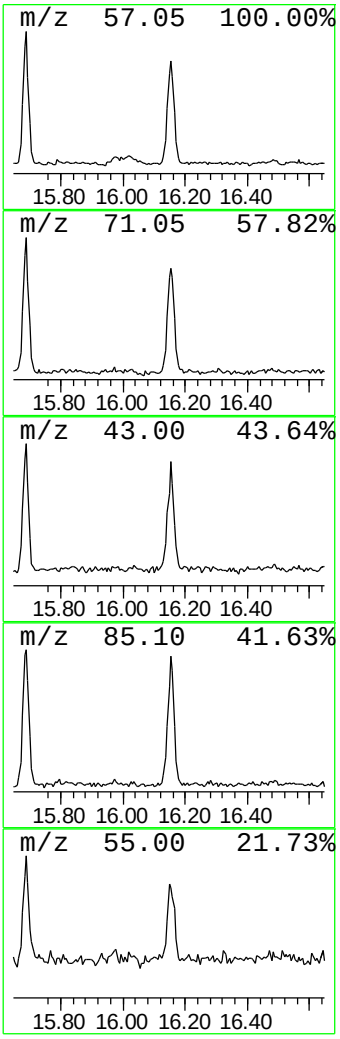
Peak Number 6 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	2.82 ng	260300	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	87
2	Nonadecane	268	C19H40	000629-92-5	86
3	Heptadecane	240	C17H36	000629-78-7	86
4	Pentacosane	352	C25H52	000629-99-2	72
5	Hexatriacontane	507	C36H74	000630-06-8	68





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Sample : J4061-10
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 071718-TIPC-F-U-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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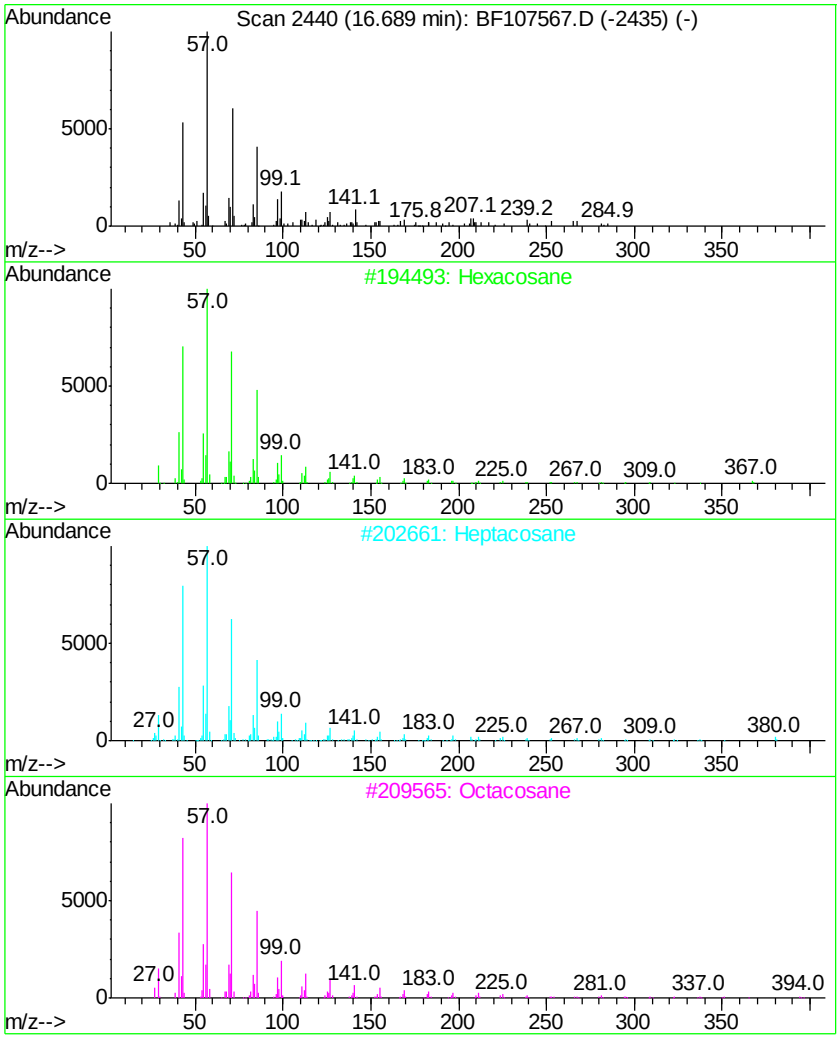
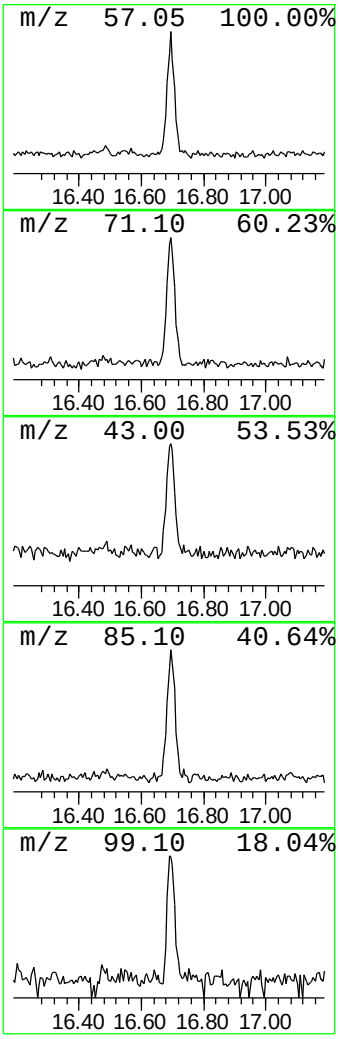
Peak Number 7 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	2.18 ng	201646	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Heptacosane	380	C27H56	000593-49-7	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Hentriacontane	437	C31H64	000630-04-6	86
5	Nonadecane	268	C19H40	000629-92-5	83





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	2.0	ng	184640	1	6.97	1832520	20.0
unknown6.74	6.74	51.8	ng	4749900	1	6.97	1832520	20.0
Triethyl citrate	10.68	3.3	ng	300158	3	10.01	1846840	20.0
Nonadecane, 2-met...	15.28	2.7	ng	248999	6	15.69	1846490	20.0
2-methyloctacosane	16.15	2.8	ng	260300	6	15.69	1846490	20.0
Hexacosane	16.69	2.2	ng	201646	6	15.69	1846490	20.0