LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082318\
Data File : BF108427.D
Acq On : 23 Aug 2018 18:16
Operator : JU/SJ
Sample : J4535-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RA-081618-FL-036

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-BF080818.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	2.390	3	9	22	rVB	463839	682446	15.33%	1.882%
2	5.254	492	496	505	rVB	181961	233406	5.24%	0.644%
3	5.631	555	560	563	rBV	3415507	3399845	76.37%	9.375%
4	6.625	722	729	732	rBV	3243857	3711857	83.38%	10.236%
5	6.772	749	754	757	rBV	3636091	3606853	81.02%	9.946%
6	6.995	789	792	796	rBV	1016592	903515	20.29%	2.492%
7	7.154	815	819	823	rBV	2907486	2626122	58.99%	7.242%
8	7.560	882	888	891	rBV	2181547	2373894	53.32%	6.546%
9	8.284	1006	1011	1014	rBV	1230831	1142892	25.67%	3.152%
10	9.354	1187	1193	1197	rBV	4174195	4259578	95.68%	11.746%
11	9.742	1256	1259	1264	rBV	268882	253424	5.69%	0.699%
12	10.042	1305	1310	1314	rBV	1533702	1367508	30.72%	3.771%
13	10.836	1440	1445	1457	rBV	2866126	3004231	67.48%	8.285%
14	11.536	1560	1564	1568	rBV	1599525	1450846	32.59%	4.001%
15	12.042	1646	1650	1653	rBV	64513	59826	1.34%	0.165%
16	13.124	1829	1834	1837	rBV	4570582	4451910	100.00%	12.277%
17	14.060	1986	1993	2005	rBV5	76003	277438	6.23%	0.765%
18	14.189	2011	2015	2019	rBV	1240073	1096292	24.63%	3.023%
19	14.318	2034	2037	2040	rVB	62852	49665	1.12%	0.137%
20	14.624	2086	2089	2094	rVB2	68421	66611	1.50%	0.184%
21	14.954	2141	2145	2148	rBV	59633	62019	1.39%	0.171%
22	15.036	2155	2159	2163	rVB	111273	112980	2.54%	0.312%
23	15.312	2202	2206	2213	rBV	61499	76815	1.73%	0.212%
24	15.742	2271	2279	2285	rBV	590644	845267	18.99%	2.331%
25	16.195	2351	2356	2362	rVB	51709	84893	1.91%	0.234%
26	16.748	2444	2450	2456	rBV	32434	62959	1.41%	0.174%

Sum of corrected areas: 36263092

LSC Report - Integrated Chromatogram

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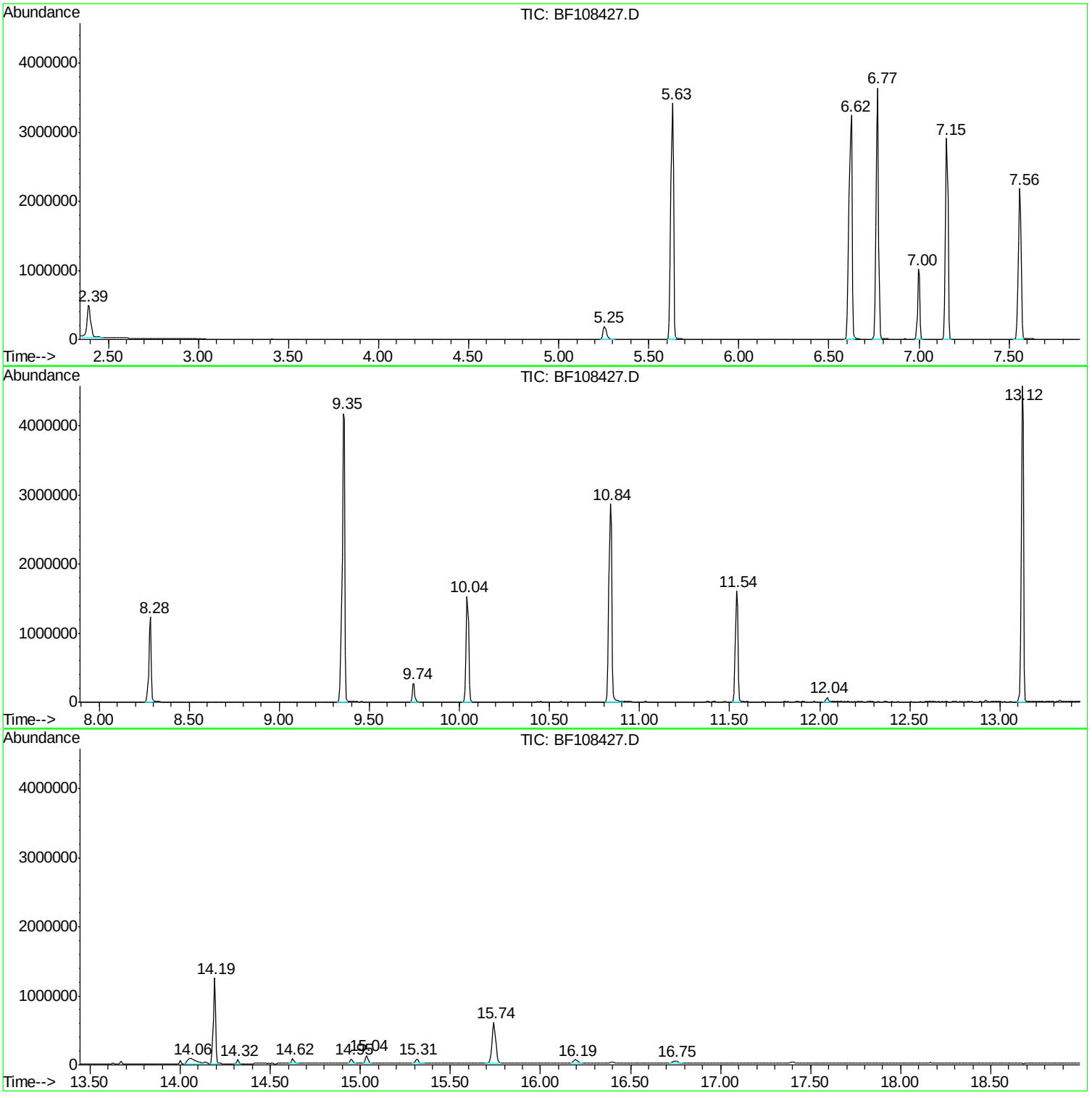
Operator : JU/SJ
Sample : J4535-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RA-081618-FL-036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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\BF082318\
Data File : BF108427.D
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Operator : JU/SJ
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Instrument : BNA_F
ClientSampleId : RA-081618-FL-036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

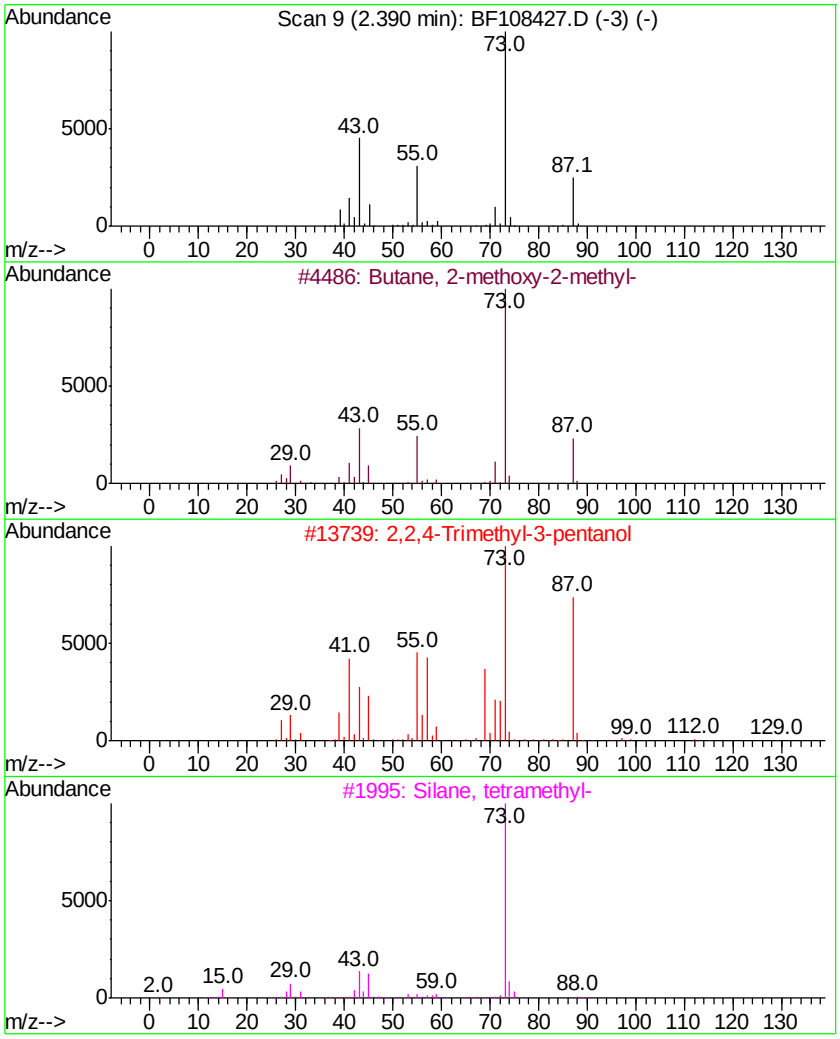
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

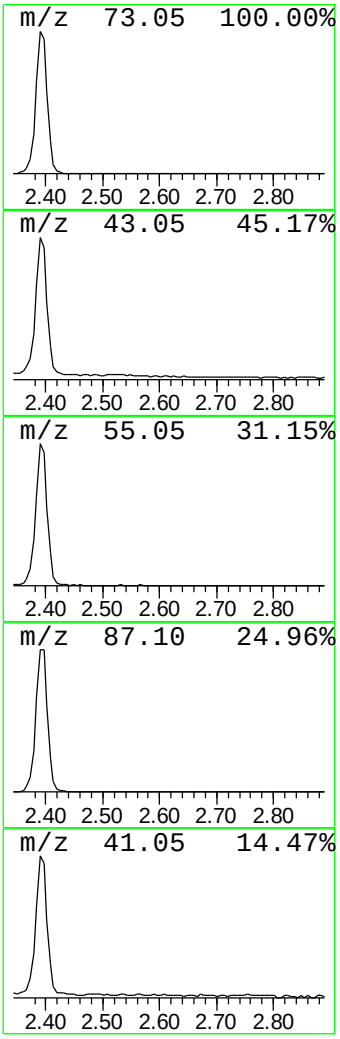
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.39	15.11 ng	682446	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Data File : BF108427.D
Acq On : 23 Aug 2018 18:16
Operator : JU/SJ
Sample : J4535-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RA-081618-FL-036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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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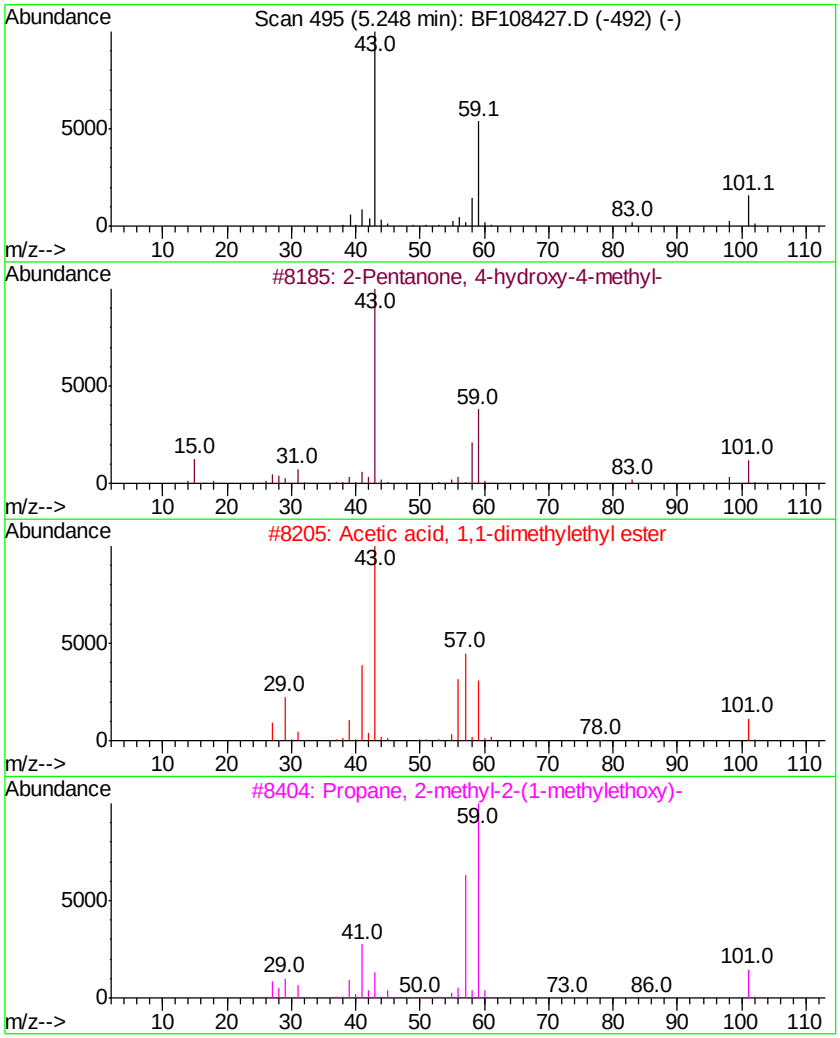
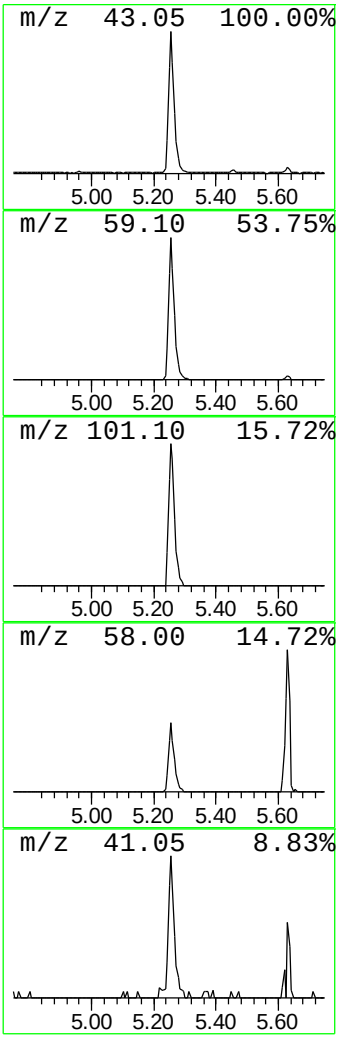
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	5.17 ng	233406	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082318\
Data File : BF108427.D
Acq On : 23 Aug 2018 18:16
Operator : JU/SJ
Sample : J4535-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RA-081618-FL-036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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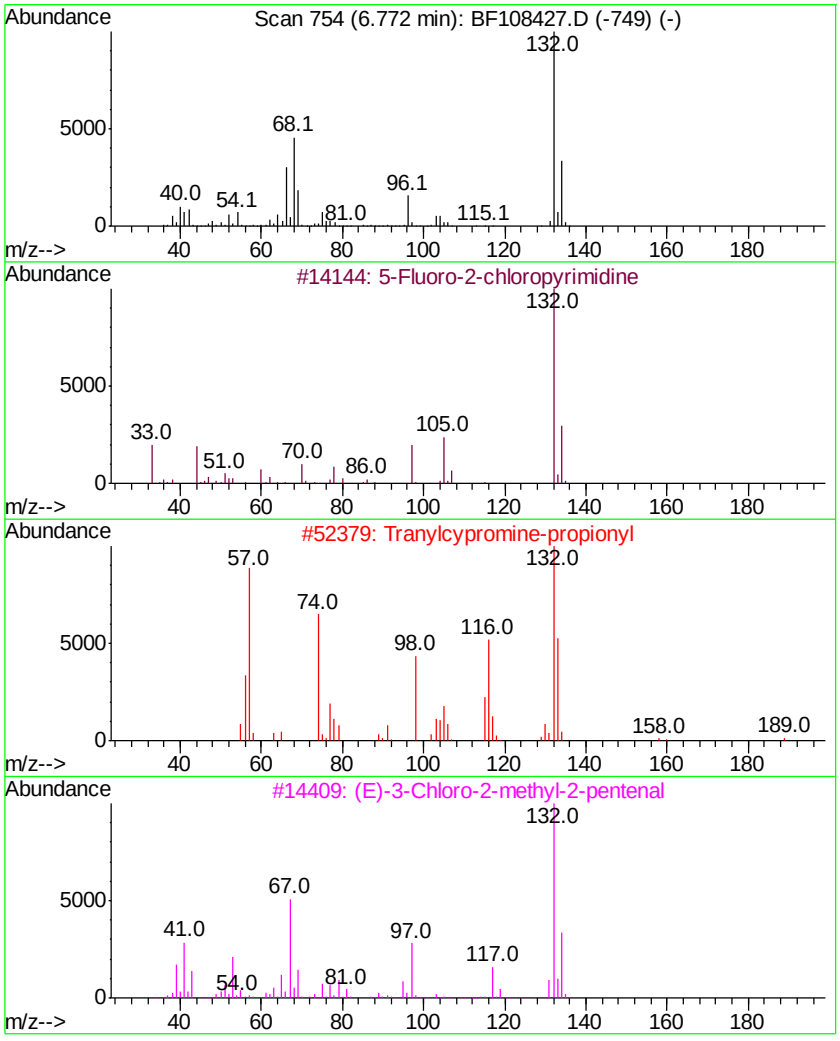
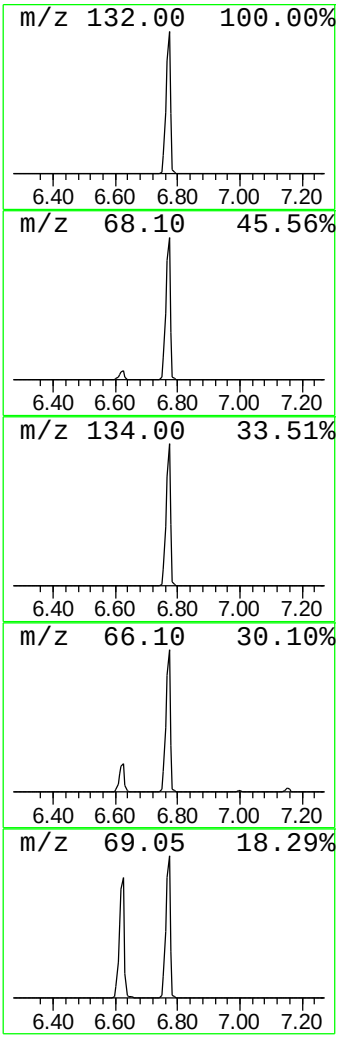
Peak Number 3 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	79.84 ng	3606850	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

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Operator : JU/SJ
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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RA-081618-FL-036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

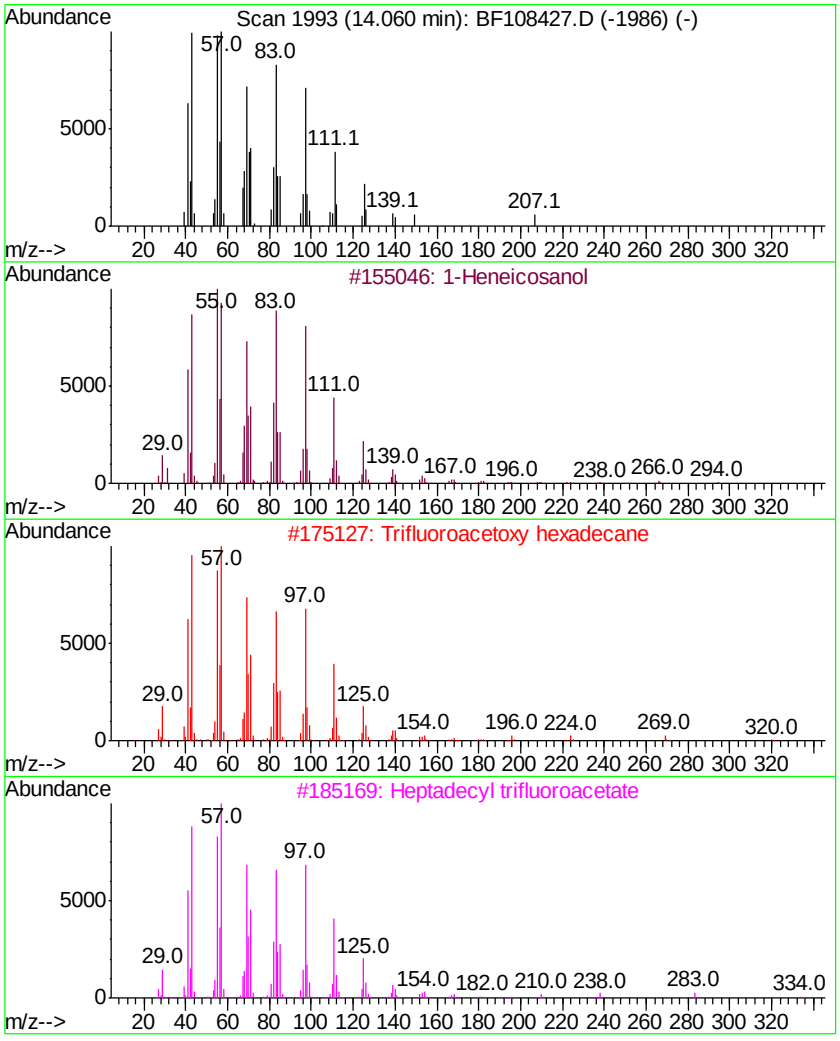
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

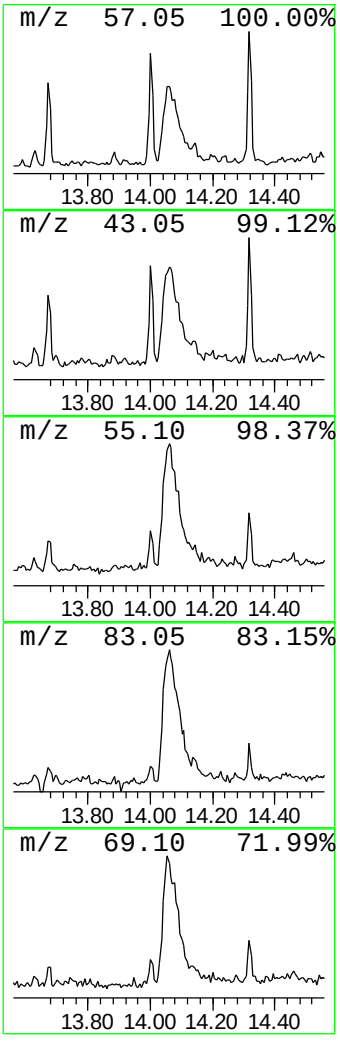
****

Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.06	5.06 ng	277438	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	95
4	1-Docosene	308	C22H44	001599-67-3	95
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082318\
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Operator : JU/SJ
Sample : J4535-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RA-081618-FL-036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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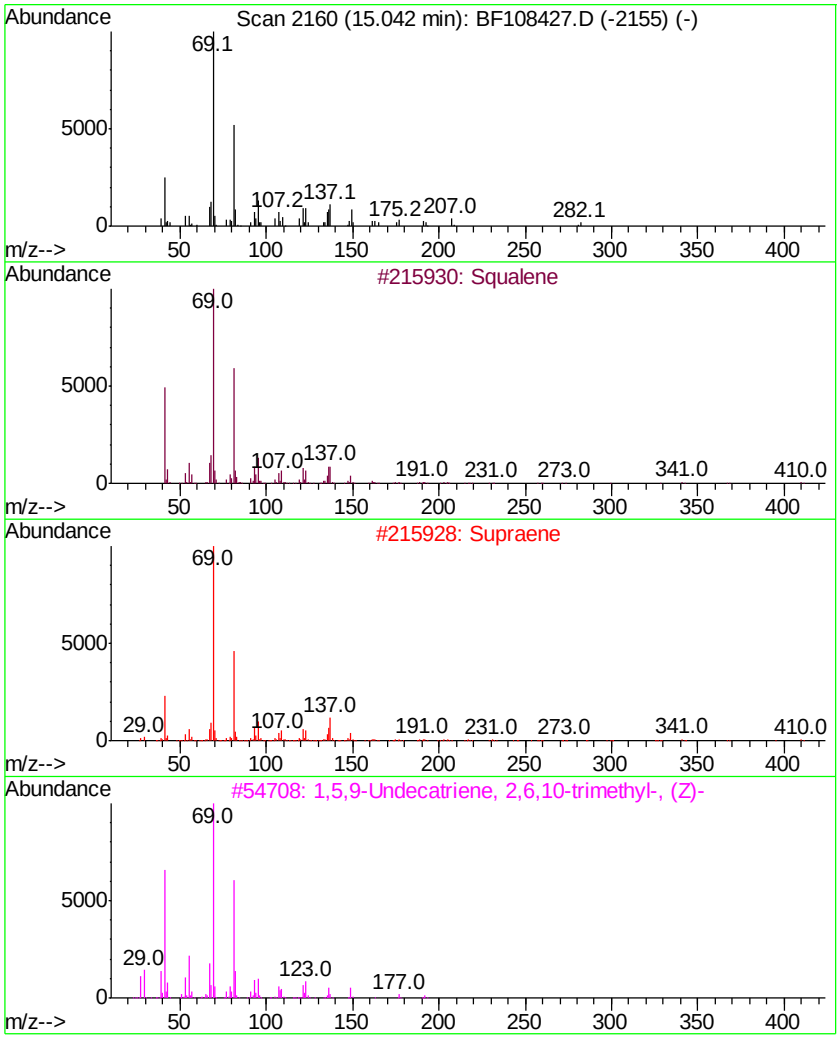
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

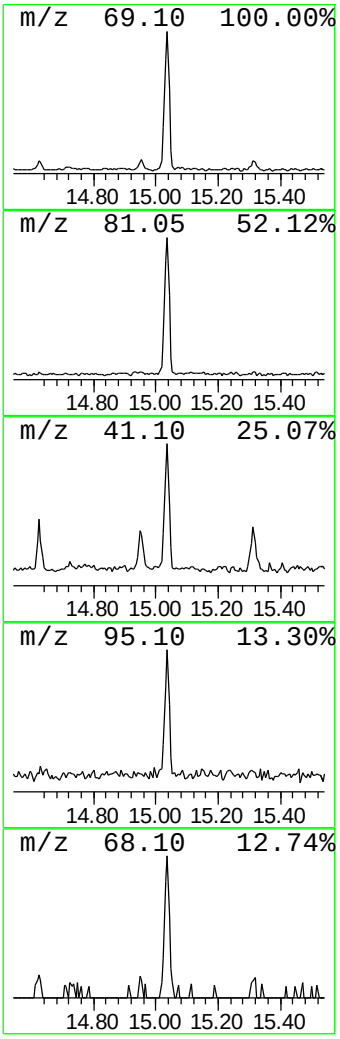
****

Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	2.67 ng	112980	Perylene-d12	15.74

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	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52





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Sample : J4535-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RA-081618-FL-036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
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TIC Library : C:\DATABASE\NIST11.L
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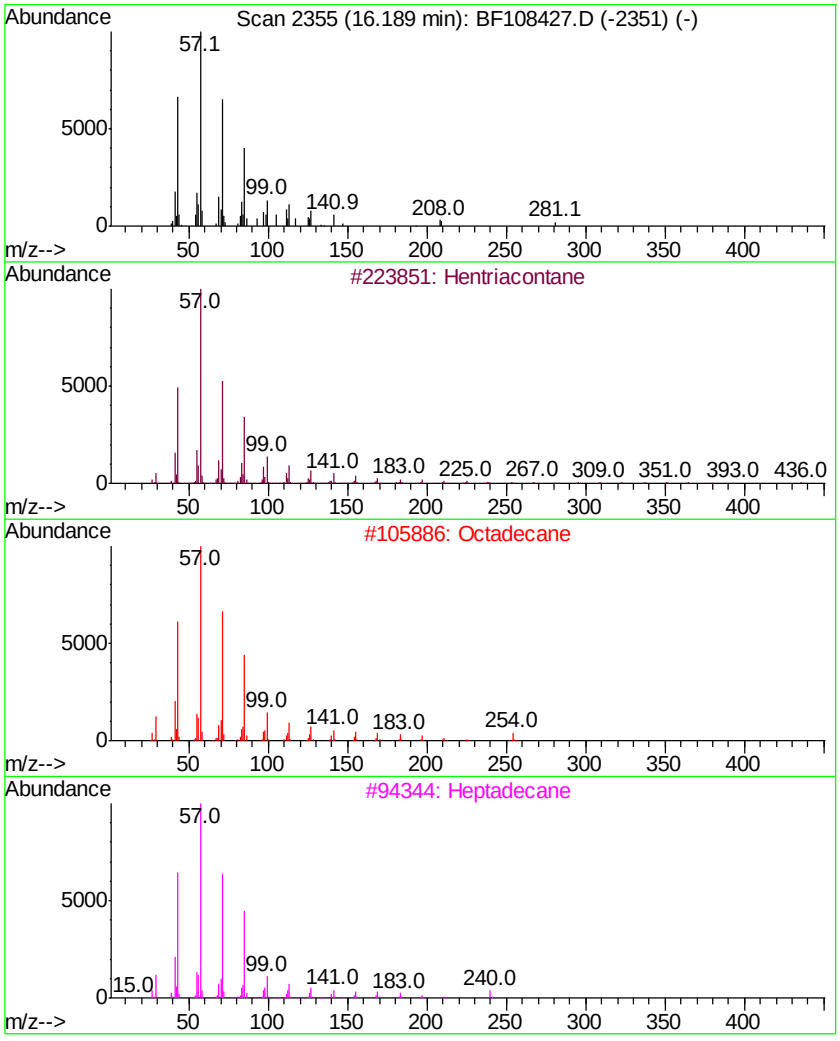
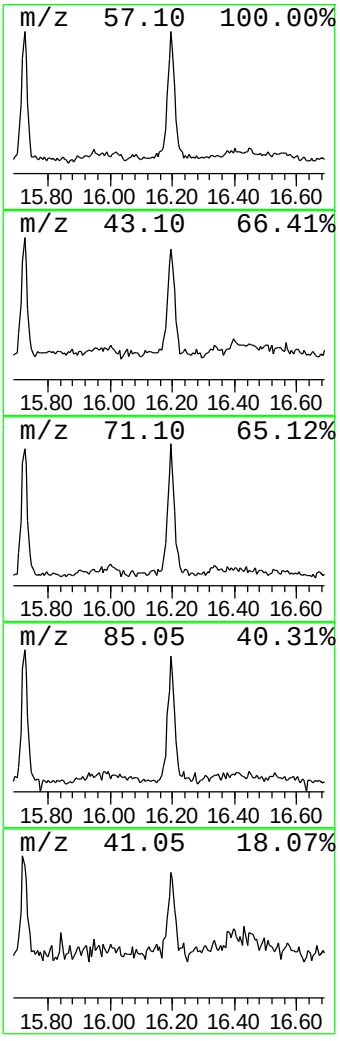
****

Peak Number 7 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.01 ng	84893	Perylene-d12	15.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Heptadecane	240	C17H36	000629-78-7	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Docosane	310	C22H46	000629-97-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082318\
Data File : BF108427.D
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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : RA-081618-FL-036

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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
Butane, 2-methoxy...	2.39	15.1	ng	682446	1	7.00	903515	20.0
2-Pentanone, 4-hy...	5.25	5.2	ng	233406	1	7.00	903515	20.0
unknown6.77	6.77	79.8	ng	3606850	1	7.00	903515	20.0
1-Heneicosanol	14.06	5.1	ng	277438	5	14.19	1096290	20.0
Squalene	15.04	2.7	ng	112980	6	15.74	845267	20.0
Hentriacontane	16.19	2.0	ng	84893	6	15.74	845267	20.0