LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101218\
Data File : BF109834.D
Acq On : 12 Oct 2018 15:31
Operator : JU/SJ
Sample : J5371-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100818-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-BF100818.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	4.887	473	476	489	rBV	62637	83057	2.01%	0.358%
2	5.310	545	548	568	rBV	426435	672273	16.28%	2.894%
3	6.339	720	723	740	rBV	242852	494513	11.98%	2.129%
4	6.463	740	744	767	rVV	1511002	1689740	40.92%	7.275%
5	6.692	780	783	805	rBV	438254	629310	15.24%	2.709%
6	6.851	805	810	838	rBV	2302254	2487921	60.25%	10.711%
7	7.263	875	880	900	rBV	1509090	2116911	51.27%	9.114%
8	7.975	997	1001	1033	rBV	646590	872172	21.12%	3.755%
9	9.051	1178	1184	1222	rBV	3715611	4129034	100.00%	17.777%
10	9.445	1248	1251	1260	rVB	53656	62159	1.51%	0.268%
11	9.722	1293	1298	1314	rBV	1024121	1040257	25.19%	4.479%
12	10.510	1428	1432	1446	rBV	1460606	1709245	41.40%	7.359%
13	11.198	1546	1549	1576	rBV	815200	1111180	26.91%	4.784%
14	11.739	1637	1641	1655	rBV2	51302	92487	2.24%	0.398%
15	12.786	1814	1819	1838	rBV	3452795	3826375	92.67%	16.474%
16	13.704	1967	1975	1985	rBV6	23891	80549	1.95%	0.347%
17	13.827	1990	1996	2015	rVV	768432	884515	21.42%	3.808%
18	14.298	2071	2076	2082	rBV2	49145	51813	1.25%	0.223%
19	14.592	2122	2126	2132	rBV	86335	87087	2.11%	0.375%
20	14.662	2134	2138	2142	rBV	47048	45051	1.09%	0.194%
21	14.904	2173	2179	2187	rBV	109001	120667	2.92%	0.520%
22	15.227	2229	2234	2251	rBV2	364685	761771	18.45%	3.280%
23	15.645	2298	2305	2314	rBV	75253	112492	2.72%	0.484%
24	16.104	2378	2383	2395	rVB	40078	66167	1.60%	0.285%

Sum of corrected areas: 23226746

LSC Report - Integrated Chromatogram

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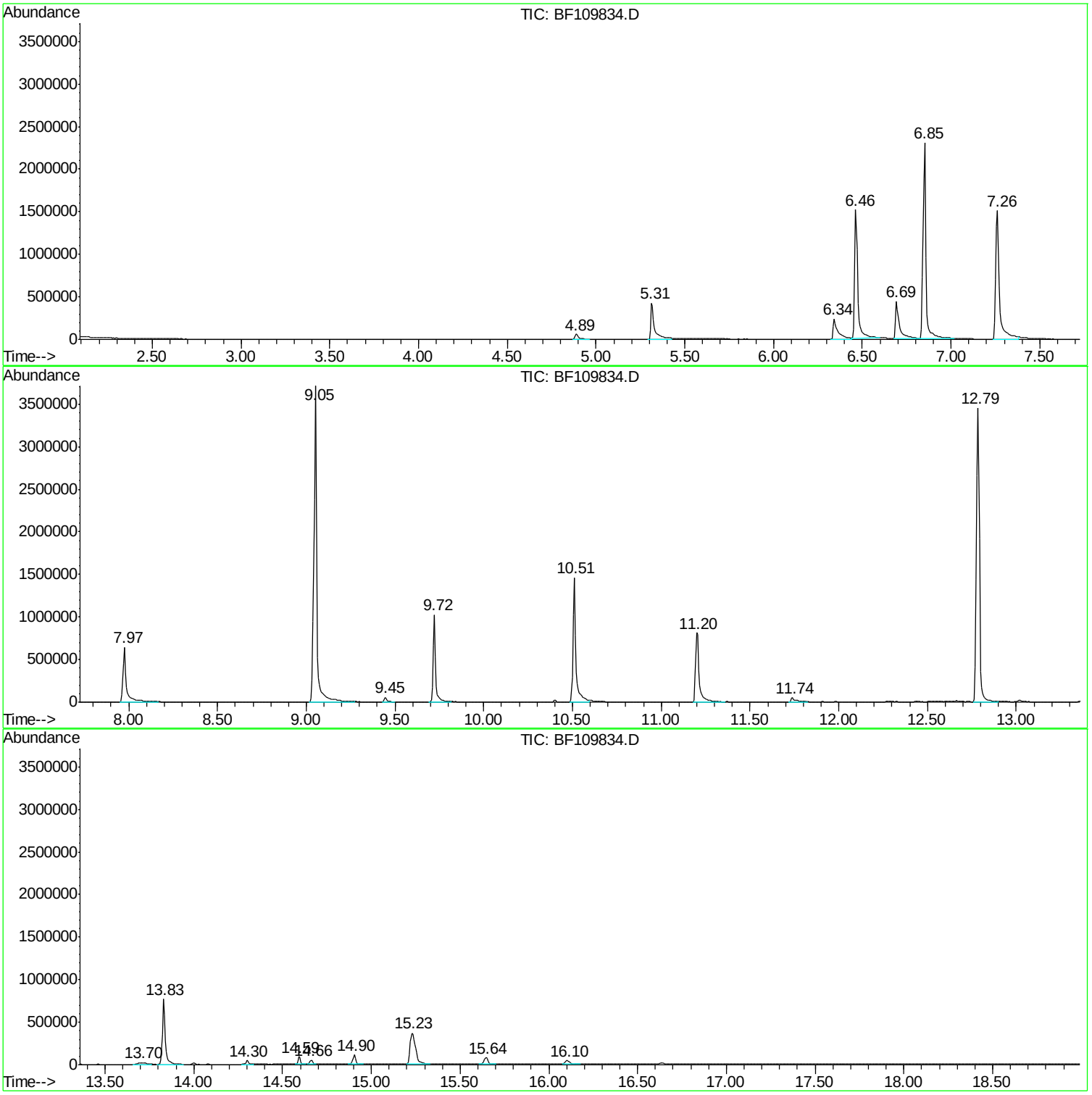
Sample : J5371-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
100818-TIPC-F-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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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Operator : JU/SJ
Sample : J5371-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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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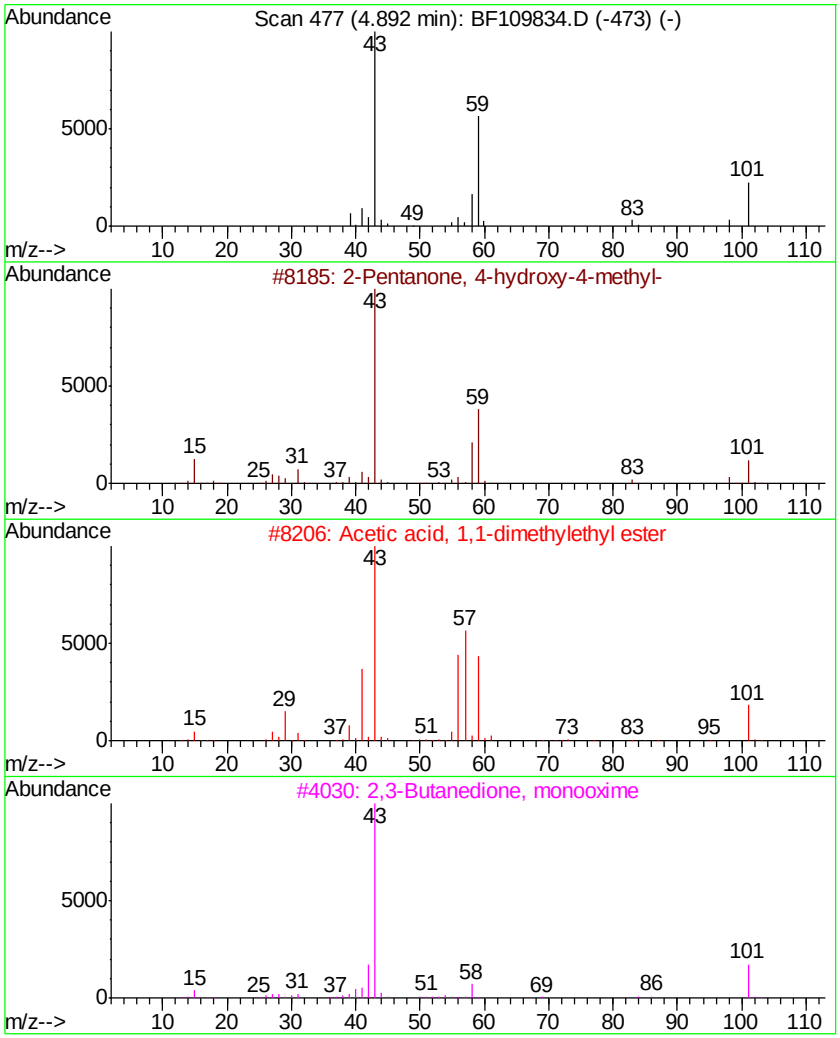
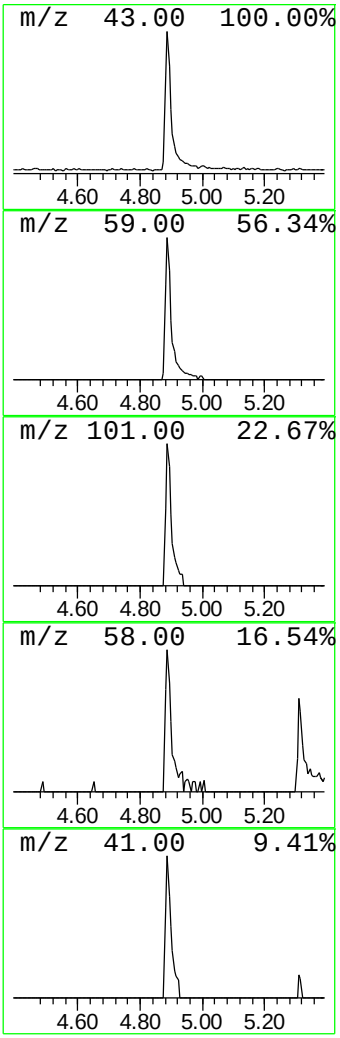
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	2.64 ng	83057	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Acetone	58	C3H6O	000067-64-1	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





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Misc :
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Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
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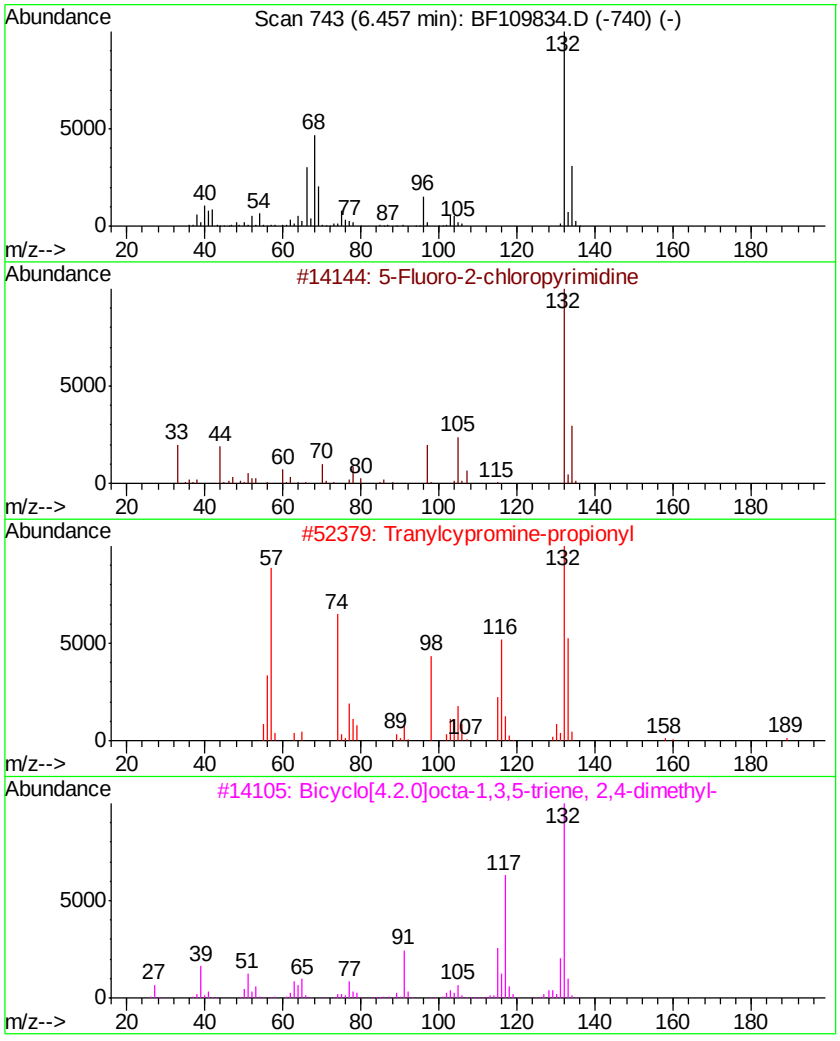
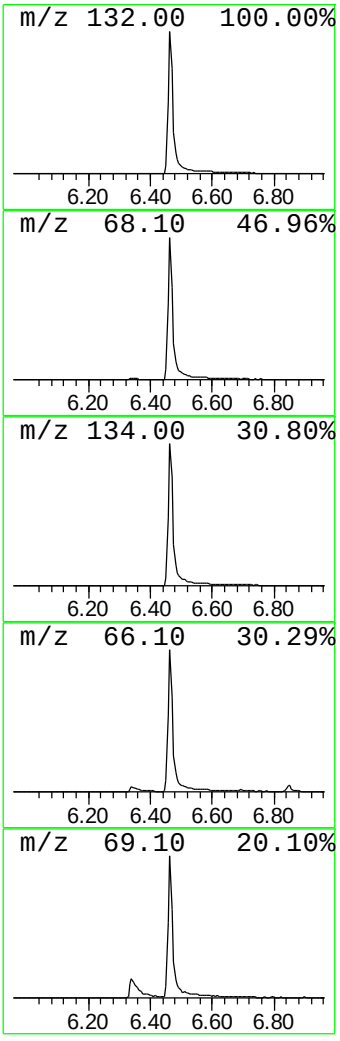
Peak Number 2 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	53.70 ng	1689740	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





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Operator : JU/SJ
Sample : J5371-10
Misc :
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Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
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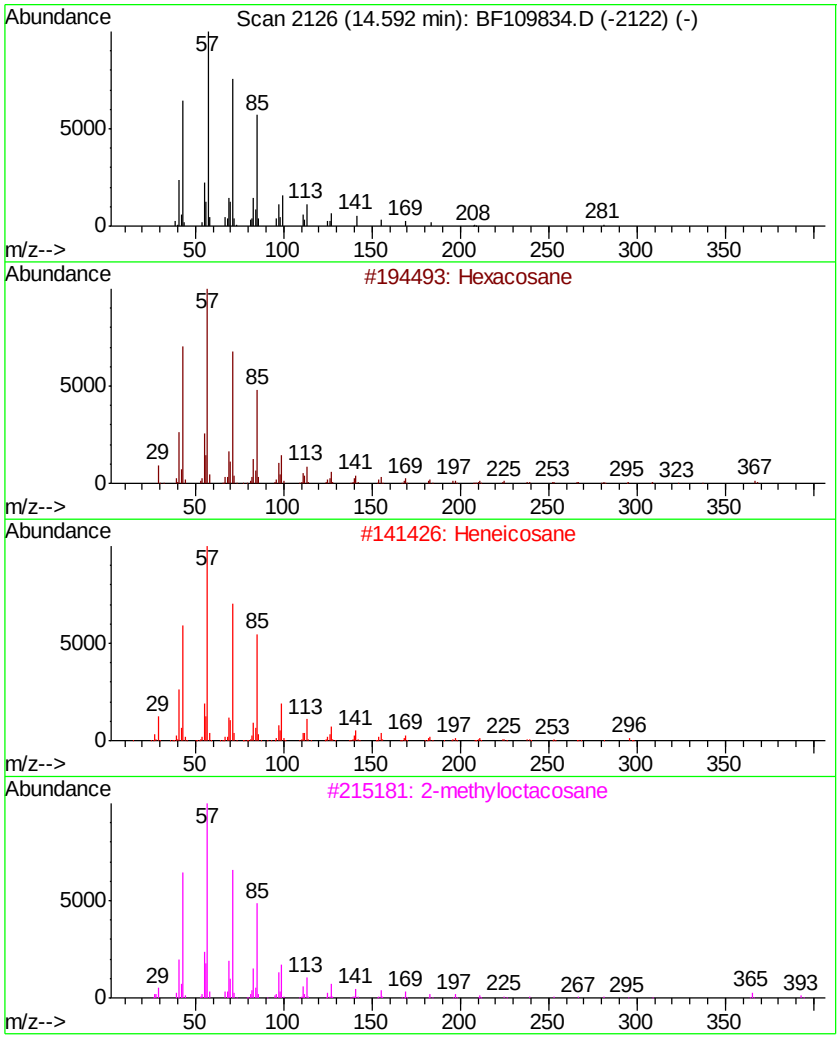
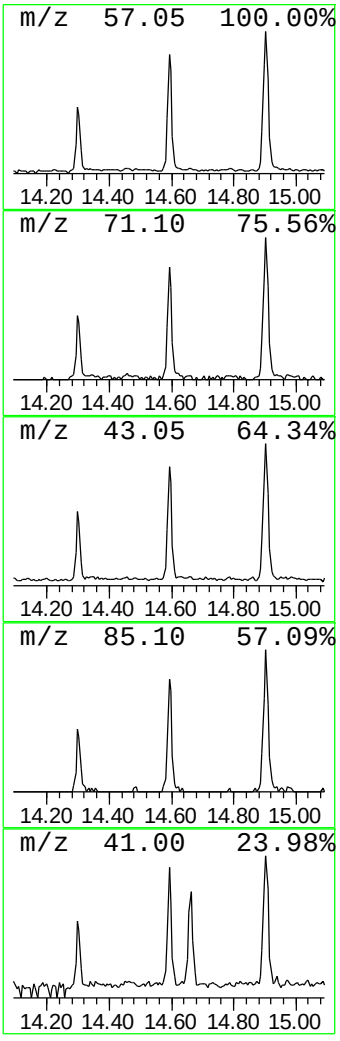
Peak Number 4 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.29 ng	87087	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
5	Heptadecane	240	C17H36	000629-78-7	90





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Sample : J5371-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
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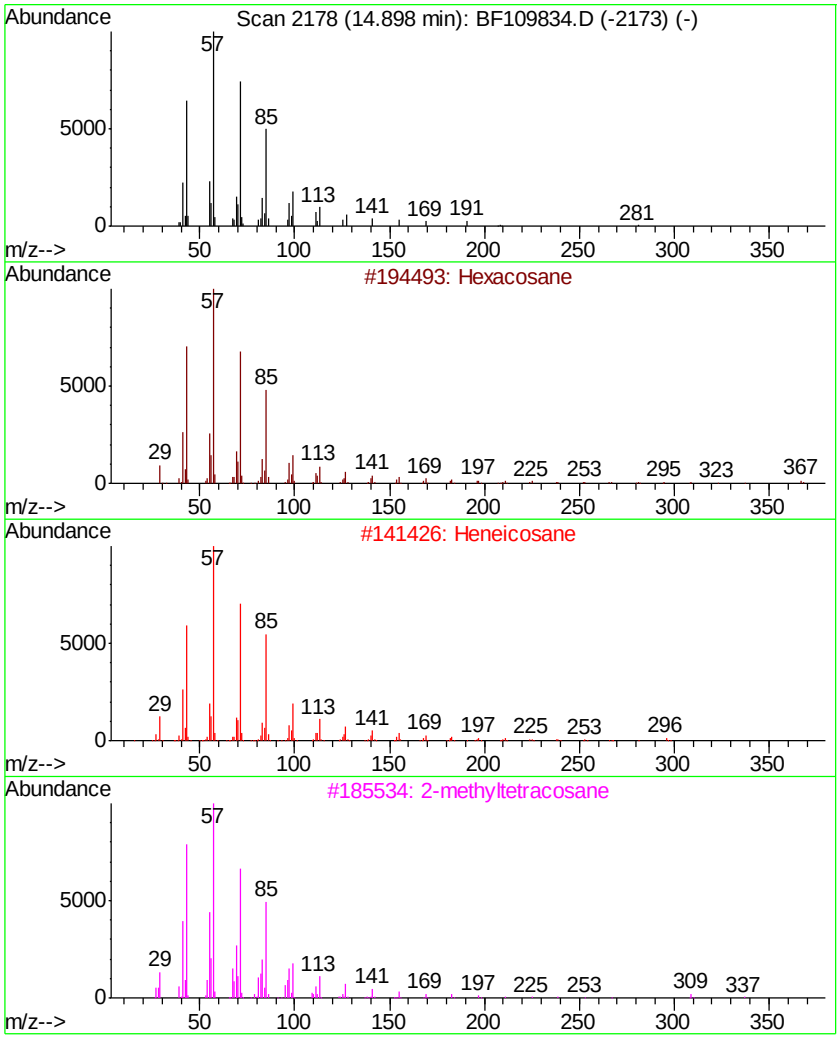
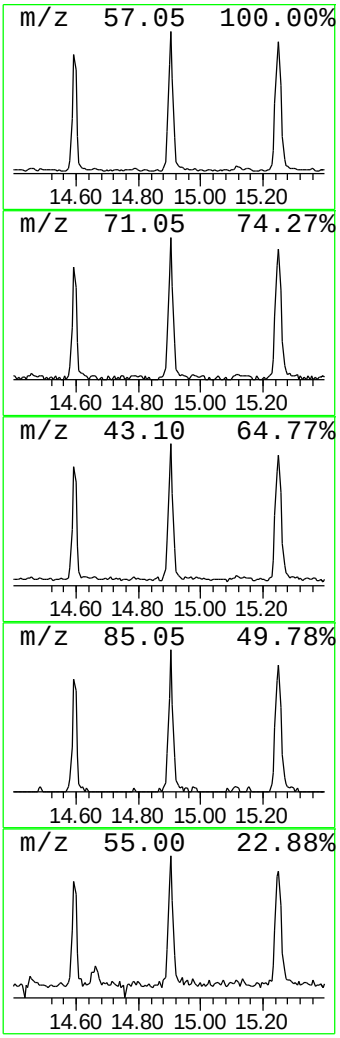
Peak Number 5 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	3.17 ng	120667	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyltetracosane	352	C25H52	1000376-72-6	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	90





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Misc :
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Instrument : BNA_F
ClientSampleId : 100818-TIPC-F-U-S

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TIC Integration Parameters: LSCINT.P

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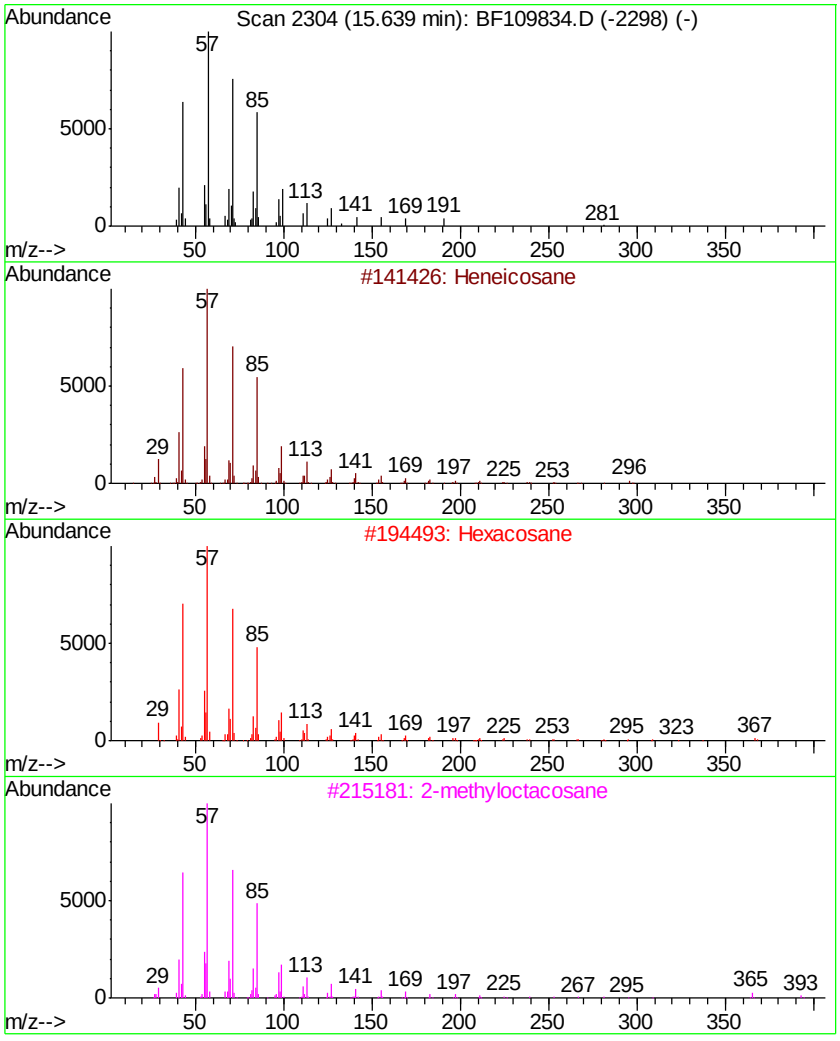
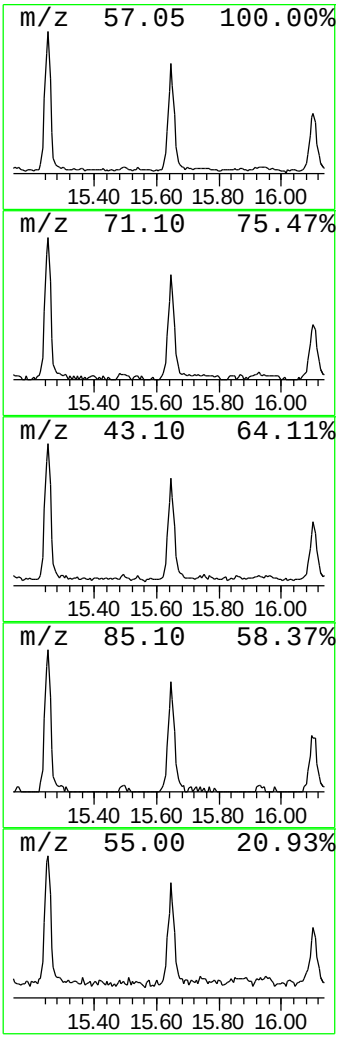
Peak Number 6 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	2.95 ng	112492	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Octacosane	394	C28H58	000630-02-4	87
5	Octadecane	254	C18H38	000593-45-3	86





Tentatively Identified Compound (LSC) summary

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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...	4.89	2.6	ng	83057	1	6.69	629310	20.0
unknown6.46	6.46	53.7	ng	1689740	1	6.69	629310	20.0
Hexacosane	14.59	2.3	ng	87087	6	15.23	761771	20.0
Heneicosane	14.90	3.2	ng	120667	6	15.23	761771	20.0
2-methyloctacosane	15.64	3.0	ng	112492	6	15.23	761771	20.0