LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062616\
Data File : BF088413.D
Acq On : 26 Jun 2016 12:37
Operator : UM/SJ
Sample : H3597-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EDD-3E

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:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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	1.690	7	9	38	rVB	317040	671452	29.72%	3.441%
2	3.164	135	138	149	rBV	23835	52496	2.32%	0.269%
3	4.684	268	271	281	rBV	76716	173153	7.66%	0.887%
4	5.130	308	310	329	rBV	939607	1612898	71.38%	8.266%
5	6.216	402	405	412	rBV	1362869	1674174	74.09%	8.580%
6	6.319	412	414	432	rVB	1699008	1818417	80.48%	9.319%
7	6.547	432	434	440	rBV	398473	425033	18.81%	2.178%
8	6.696	445	447	450	rBV	1095062	1466750	64.91%	7.517%
9	7.119	482	484	487	rBV	708440	1082513	47.91%	5.548%
10	7.828	544	546	549	rBV	414916	568807	25.17%	2.915%
11	8.913	638	641	643	rBV	2147527	2259558	100.00%	11.580%
12	9.313	674	676	678	rBV	511443	445837	19.73%	2.285%
13	9.531	692	695	696	rBV	18400	23269	1.03%	0.119%
14	9.576	696	699	702	rBV	754608	714446	31.62%	3.661%
15	10.022	736	738	740	rVB	69909	56871	2.52%	0.291%
16	10.239	754	757	760	rBV	25012	37322	1.65%	0.191%
17	10.365	766	768	777	rBV	1000143	1099039	48.64%	5.632%
18	10.491	777	779	786	rVB	94938	110720	4.90%	0.567%
19	10.936	816	818	819	rBV	53800	46084	2.04%	0.236%
20	11.051	826	828	833	rBV	704412	711894	31.51%	3.648%
21	12.262	932	934	940	rVB	18927	24224	1.07%	0.124%
22	12.468	950	952	955	rBV2	55511	74206	3.28%	0.380%
23	12.548	955	959	961	rVB	19880	25887	1.15%	0.133%
24	12.639	964	967	969	rBV	1846176	2209798	97.80%	11.325%
25	13.165	1011	1013	1015	rBV	27418	27966	1.24%	0.143%
26	13.542	1043	1046	1054	rBV	185712	354758	15.70%	1.818%
27	13.680	1055	1058	1066	rVB	568693	774914	34.29%	3.971%
28	14.182	1097	1102	1106	rBV2	11718	32262	1.43%	0.165%
29	14.548	1127	1134	1144	rBV3	16395	91753	4.06%	0.470%
30	15.028	1174	1176	1186	rVB	427536	616358	27.28%	3.159%
31	15.394	1206	1208	1211	rBV	22913	29443	1.30%	0.151%
32	15.463	1211	1214	1220	rBV4	21121	73910	3.27%	0.379%
33	15.794	1240	1243	1249	rVB2	23298	41446	1.83%	0.212%
34	16.263	1281	1284	1289	rBV2	14413	30569	1.35%	0.157%

LSC Area Percent Report

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Acq On : 26 Jun 2016 12:37
Operator : UM/SJ
Sample : H3597-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EDD-3E

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:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.377	1291	1294	1303	rVB7	6366	26731	1.18%	0.137%
36	16.811	1329	1332	1339	rVB	12150	27657	1.22%	0.142%

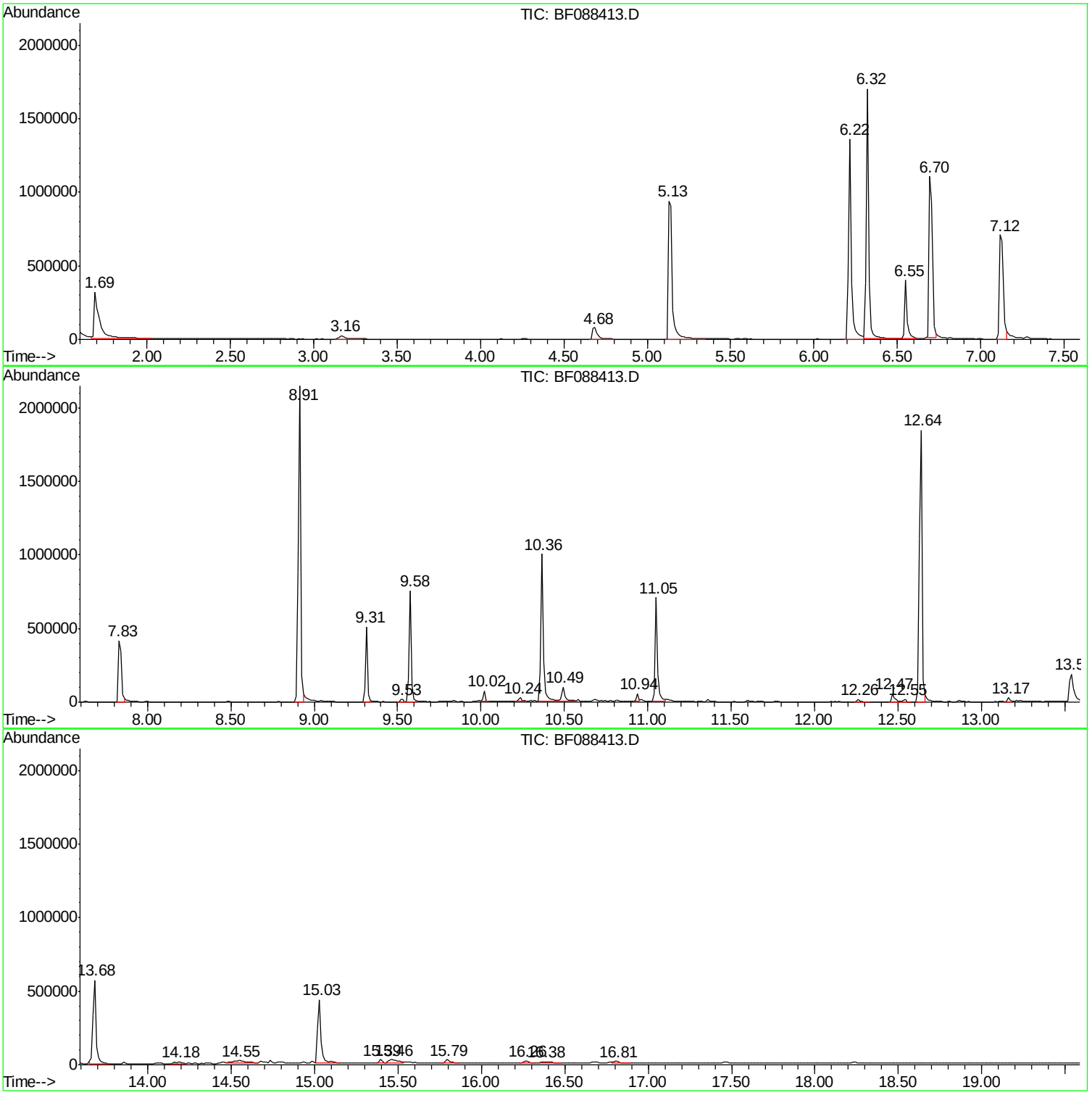
Sum of corrected areas: 19512615

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062616\
Data File : BF088413.D
Acq On : 26 Jun 2016 12:37
Operator : UM/SJ
Sample : H3597-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EDD-3E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062616\
Data File : BF088413.D
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Operator : UM/SJ
Sample : H3597-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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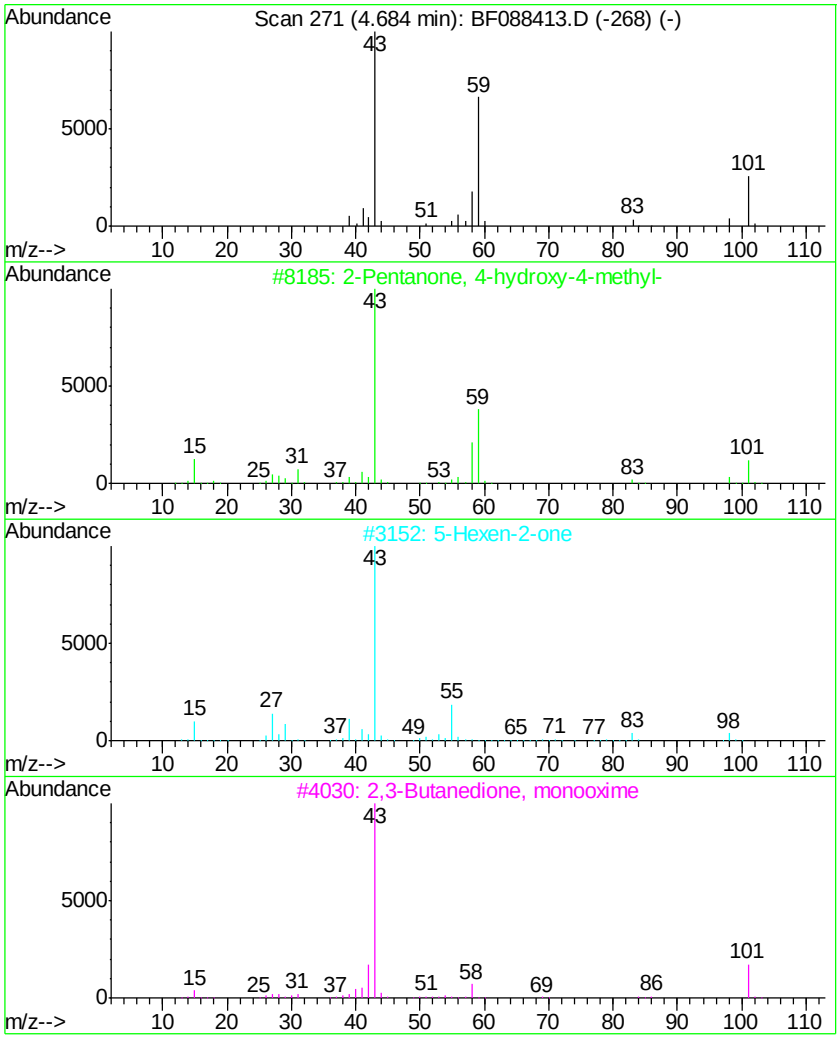
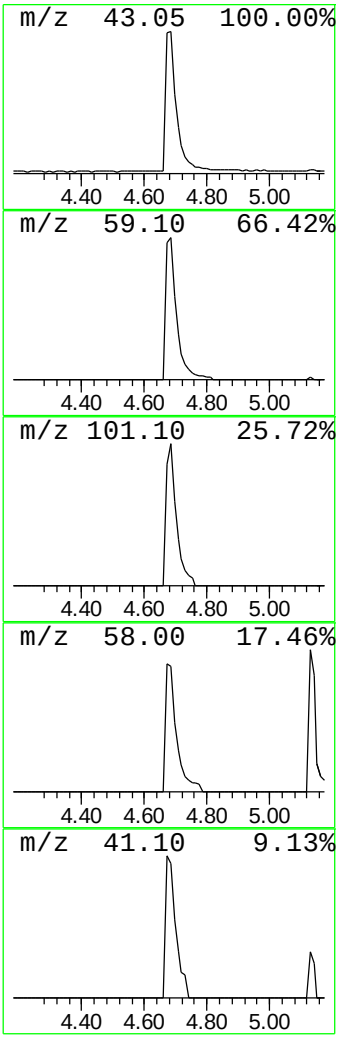
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	8.15 ng	173153	1,4-Dichlorobenzene-d4	6.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	10
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062616\
Data File : BF088413.D
Acq On : 26 Jun 2016 12:37
Operator : UM/SJ
Sample : H3597-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EDD-3E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

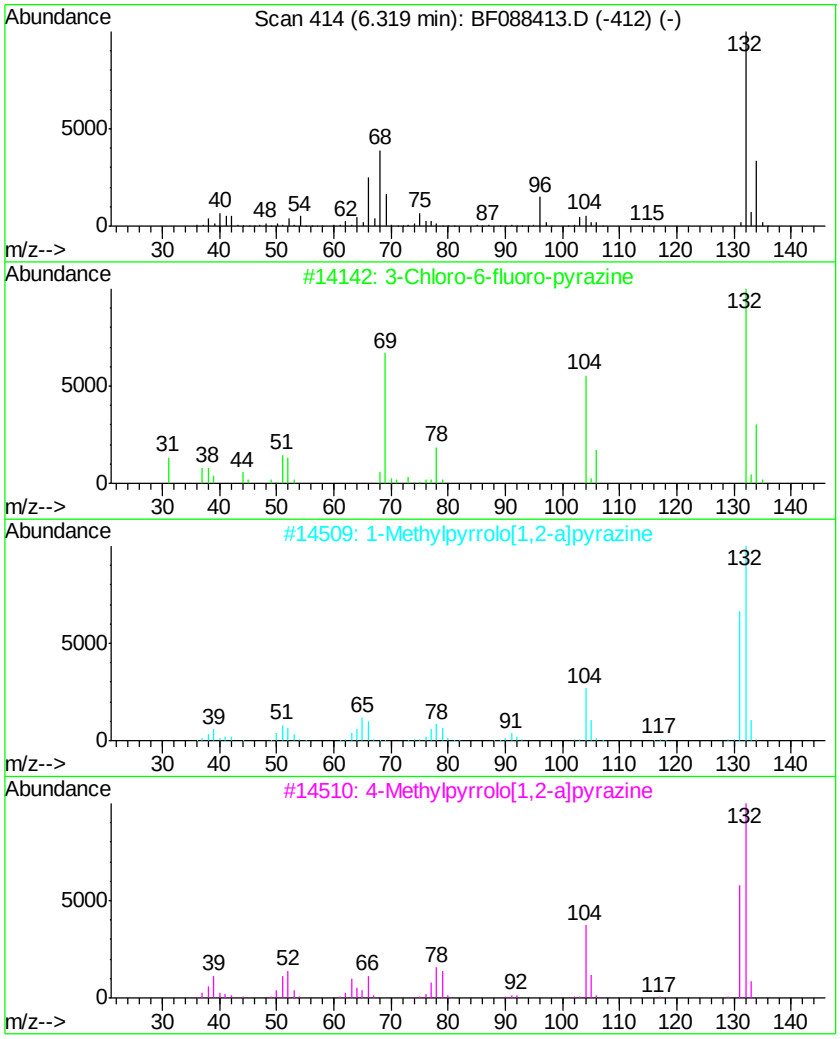
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

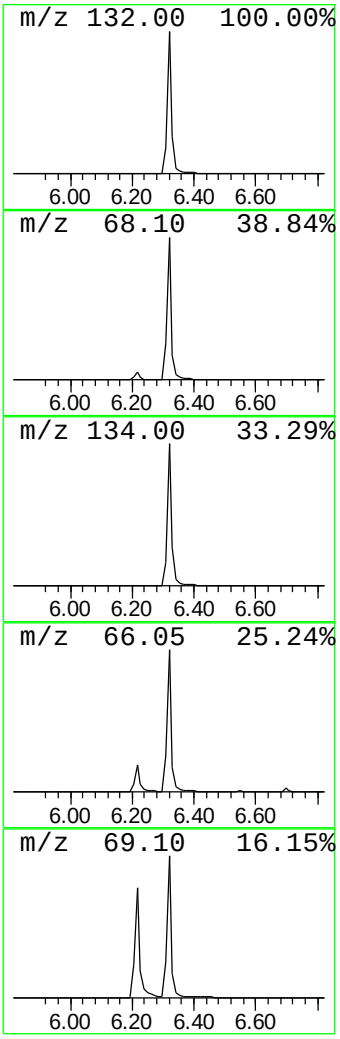
****

Peak Number 4 unknown6.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.32	85.57 ng	1818420	1,4-Dichlorobenzene-d4	6.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062616\
Data File : BF088413.D
Acq On : 26 Jun 2016 12:37
Operator : UM/SJ
Sample : H3597-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EDD-3E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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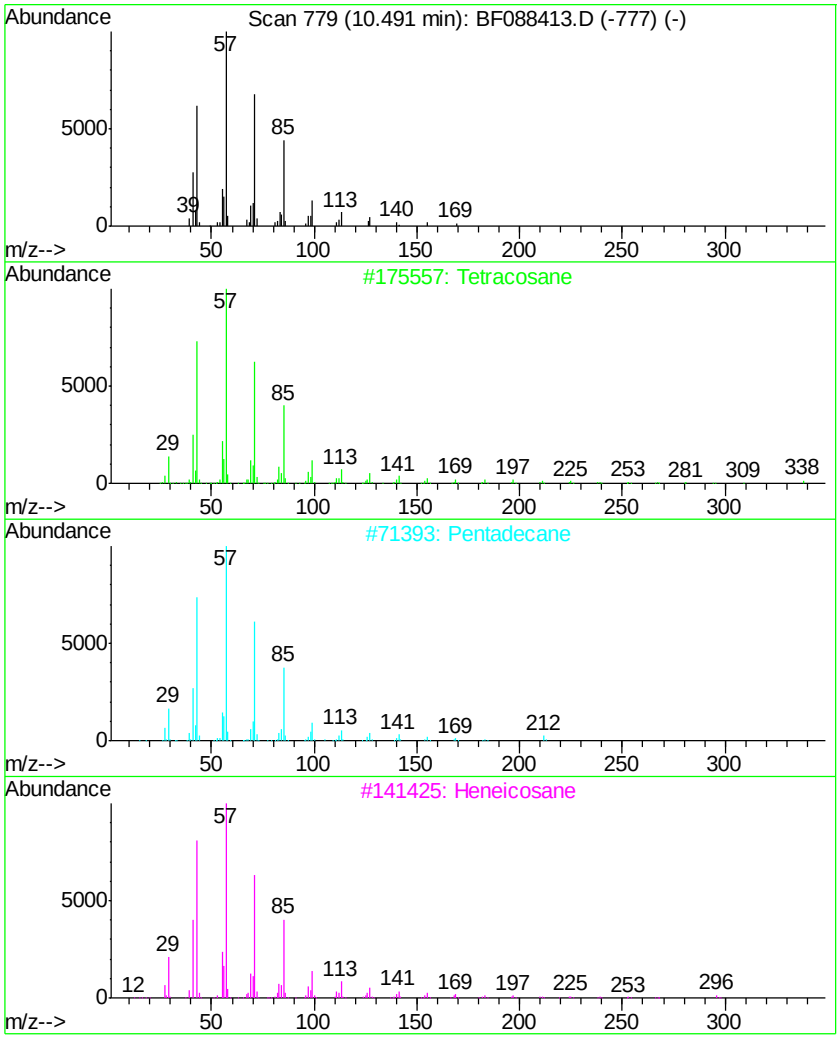
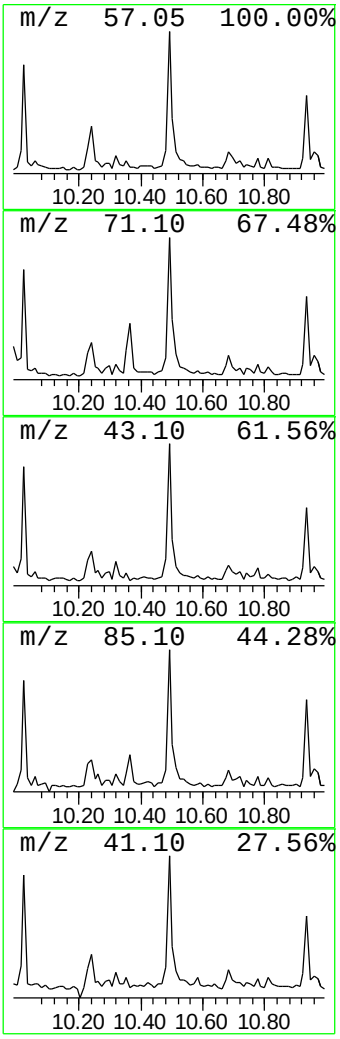
Peak Number 6 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.49	3.11 ng	110720	Phenanthrene-d10	11.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Pentadecane	212	C15H32	000629-62-9	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Hexadecane	226	C16H34	000544-76-3	90
5	Heptadecane	240	C17H36	000629-78-7	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062616\
Data File : BF088413.D
Acq On : 26 Jun 2016 12:37
Operator : UM/SJ
Sample : H3597-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EDD-3E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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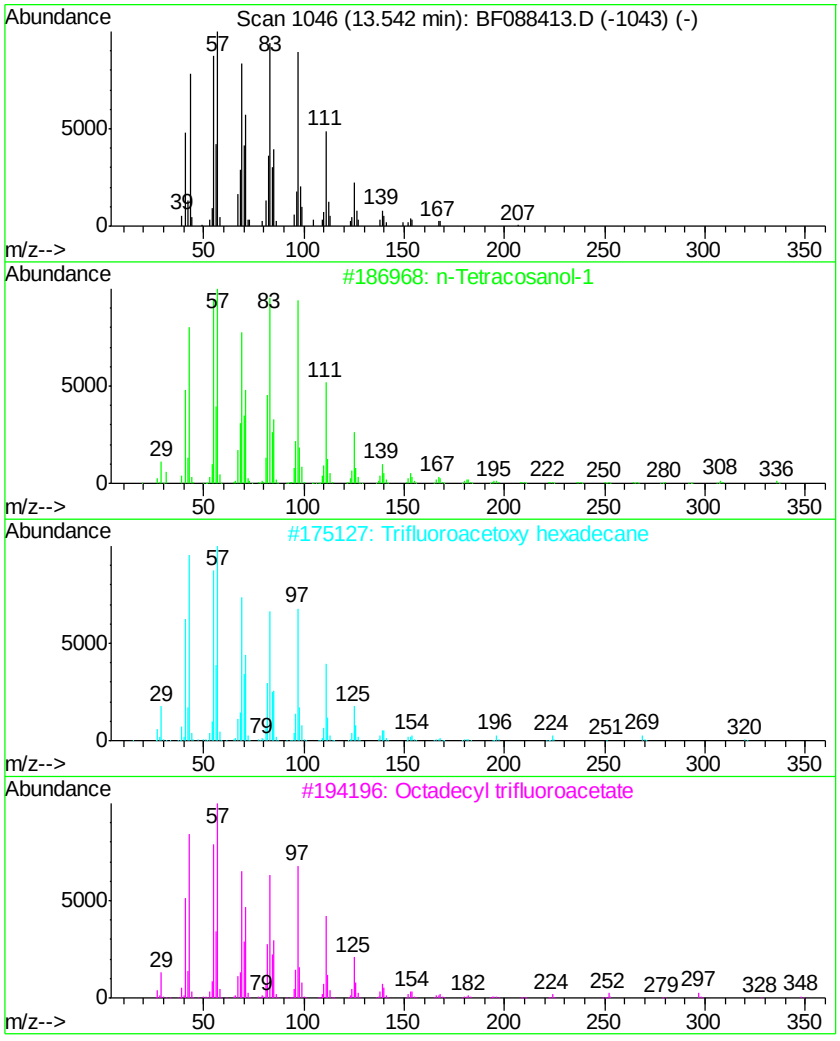
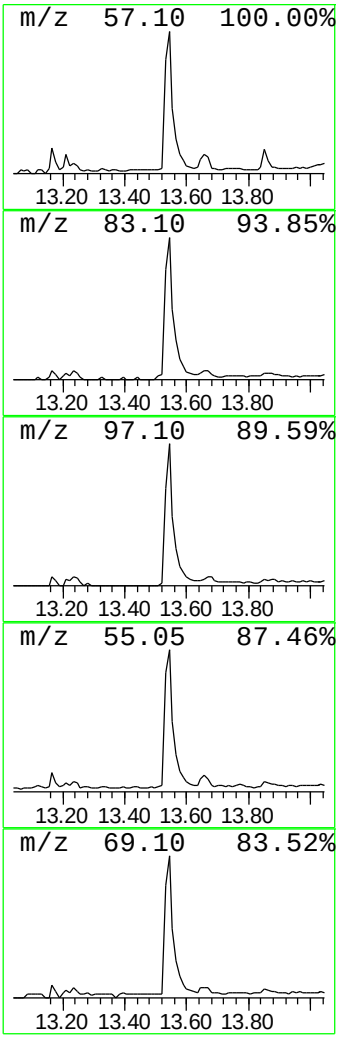
Peak Number 7 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	9.16 ng	354758	Chrysene-d12	13.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93





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Operator : UM/SJ
Sample : H3597-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EDD-3E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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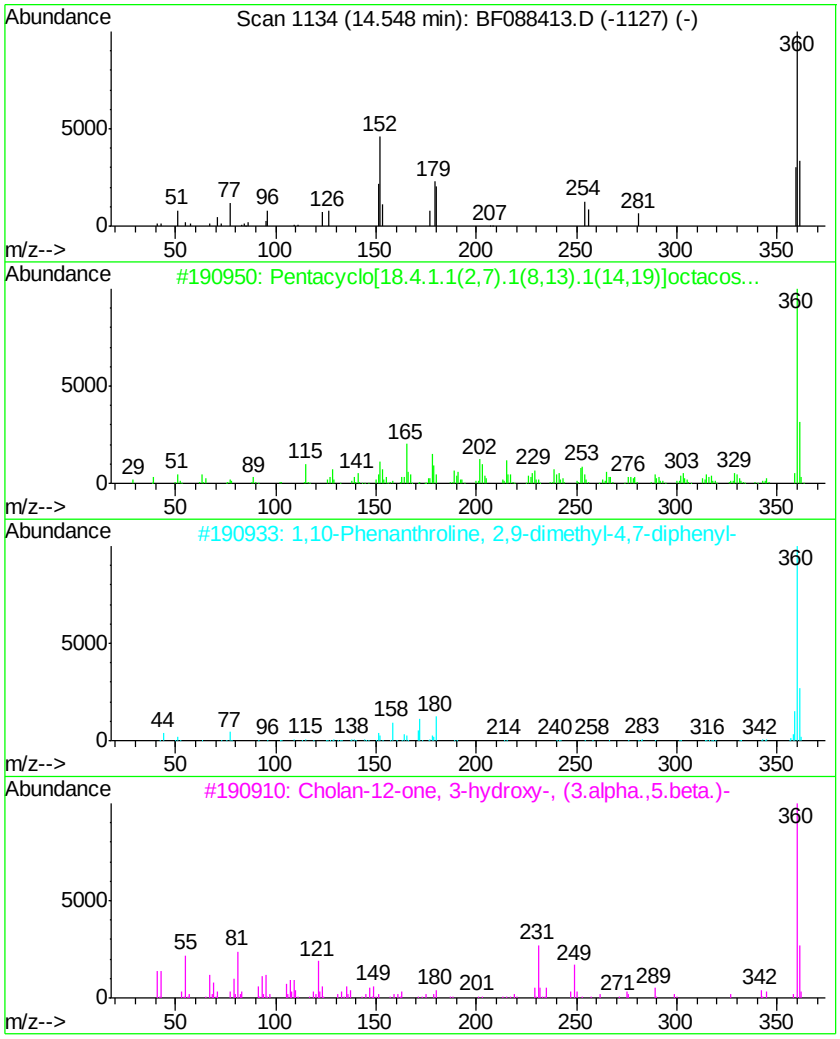
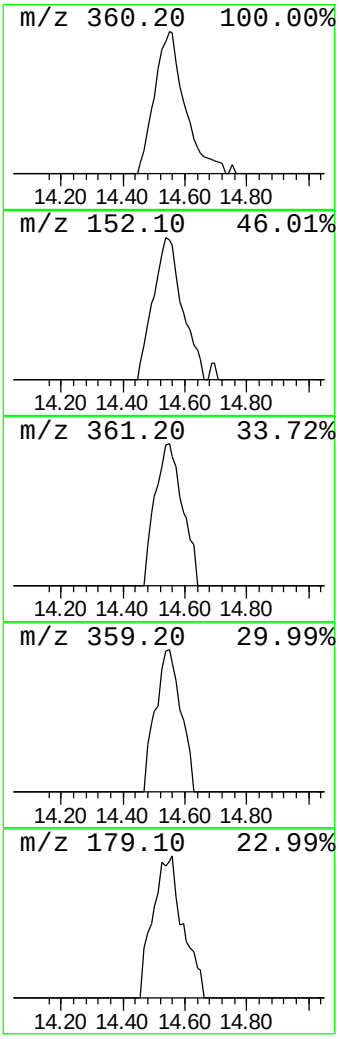
Peak Number 8 unknown14.55 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	2.98 ng	91753	Perylene-d12	15.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacyclo[18.4.1.1(2,7).1(8,13)...	360	C28H24	101077-60-5	5
2	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	5
3	Cholan-12-one, 3-hydroxy-, (3.al...	360	C24H40O2	054411-58-4	5
4	2-Cyclohexylamino-3-methyl(phenyl...	360	C23H24N2O2	134614-17-8	5
5	Melatonin, pentafluoropropionyl ...	360	C16H13F5N2O2	066012-87-1	5





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062616\
Data File : BF088413.D
Acq On : 26 Jun 2016 12:37
Operator : UM/SJ
Sample : H3597-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EDD-3E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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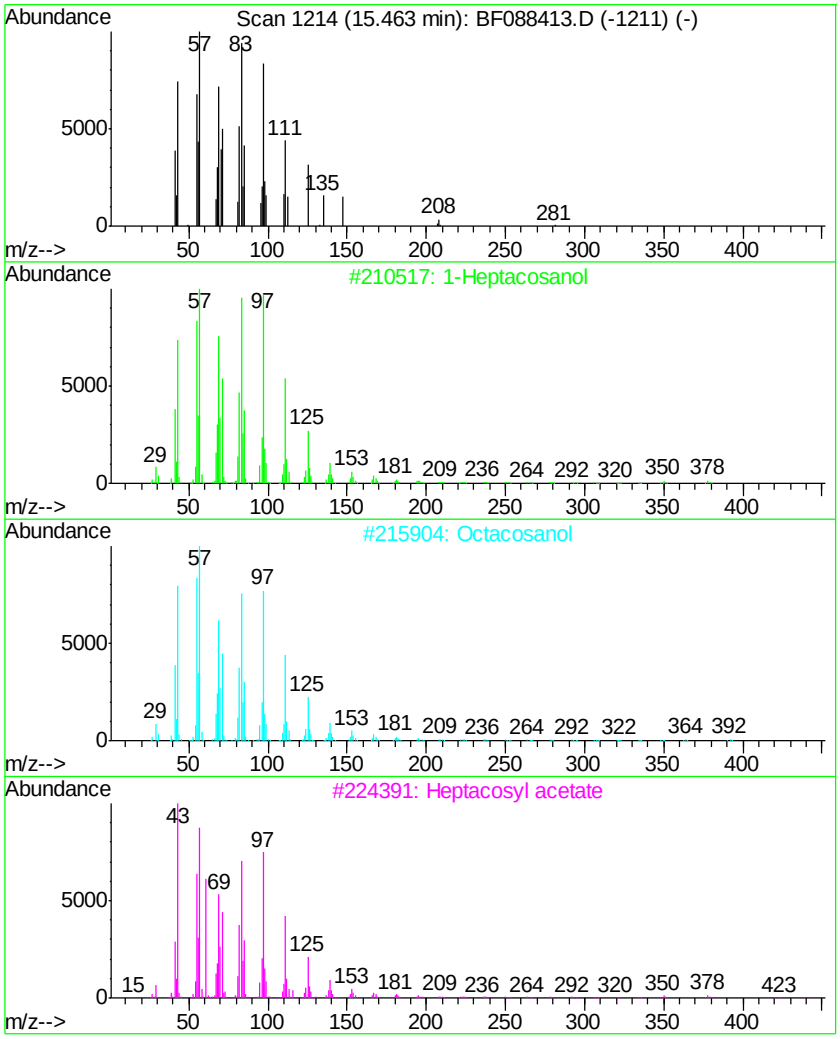
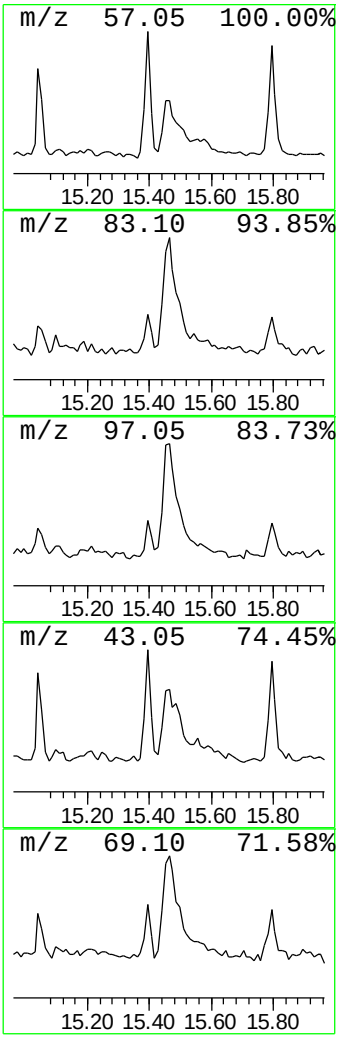
Peak Number 9 1-Heptacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.46	2.40 ng	73910	Perylene-d12	15.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	Octacosanol	410	C28H58O	000557-61-9	91
3	Heptacosyl acetate	438	C29H58O2	1000351-78-2	91
4	Triacontyl acetate	480	C32H64O2	041755-58-2	90
5	1-Heneicosanol	312	C21H44O	015594-90-8	87





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...	4.68	8.2	ng	173153	1	6.55	425033	20.0
unknown6.32	6.32	85.6	ng	1818420	1	6.55	425033	20.0
Tetracosane	10.49	3.1	ng	110720	4	11.05	711894	20.0
n-Tetracosanol-1	13.54	9.2	ng	354758	5	13.68	774914	20.0
unknown14.55	14.55	3.0	ng	91753	6	15.03	616358	20.0
1-Heptacosanol	15.46	2.4	ng	73910	6	15.03	616358	20.0