LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089056.D
Acq On : 16 Jul 2016 15:40
Operator : UM/SJ
Sample : H3989-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B2(0-5)C

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-BF063016.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	1.656	4	6	14	rVB	24317	63757	4.89%	0.496%
2	1.770	14	16	48	rVB	756380	1303379	100.00%	10.146%
3	4.787	277	280	288	rVB	96174	126618	9.71%	0.986%
4	5.256	318	321	323	rBV	764475	952119	73.05%	7.412%
5	6.319	411	414	416	rBV	1121338	1169107	89.70%	9.101%
6	6.433	422	424	426	rBV	1243918	1069298	82.04%	8.324%
7	6.662	442	444	446	rBB	450004	363384	27.88%	2.829%
8	6.822	455	458	460	rBB	838390	817579	62.73%	6.364%
9	7.233	491	494	496	rBV	564407	658587	50.53%	5.127%
10	7.953	554	557	559	rBV	363535	455248	34.93%	3.544%
11	9.028	648	651	653	rBV	1339754	1132776	86.91%	8.818%
12	9.428	684	686	688	rBV	252262	203966	15.65%	1.588%
13	9.702	707	710	712	rBV	517604	470547	36.10%	3.663%
14	10.148	748	749	751	rVB	18367	13970	1.07%	0.109%
15	10.491	776	779	781	rBV2	414177	491494	37.71%	3.826%
16	10.616	788	790	794	rVB	18035	28991	2.22%	0.226%
17	11.062	827	829	831	rBV	16583	21595	1.66%	0.168%
18	11.176	837	839	840	rBV	481260	397219	30.48%	3.092%
19	11.245	843	845	847	rVB	18317	26340	2.02%	0.205%
20	11.497	864	867	869	rVB	14061	17275	1.33%	0.134%
21	11.679	876	883	884	rBV	15804	23755	1.82%	0.185%
22	11.702	884	885	888	rVV	16416	19968	1.53%	0.155%
23	11.782	891	892	896	rVV2	24277	36437	2.80%	0.284%
24	11.999	906	911	913	rBV2	12296	23877	1.83%	0.186%
25	12.159	919	925	926	rBV5	5106	16755	1.29%	0.130%
26	12.228	928	931	932	rBV	13863	18201	1.40%	0.142%
27	12.388	943	945	947	rVB	124804	169434	13.00%	1.319%
28	12.605	962	964	967	rBV	164187	186965	14.34%	1.455%
29	12.662	967	969	972	rVB3	9013	20370	1.56%	0.159%
30	12.765	976	978	980	rVB	861847	816178	62.62%	6.354%
31	12.834	980	984	985	rBV	14541	17225	1.32%	0.134%
32	12.914	988	991	992	rBV3	16751	32832	2.52%	0.256%
33	12.937	992	993	995	rVB	27693	25669	1.97%	0.200%
34	13.005	995	999	1001	rBV	26552	44107	3.38%	0.343%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : Q7-B2(0-5)C

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
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.040	1001	1002	1008	rBV2	21524	38379	2.94%	0.299%
36	13.131	1008	1010	1011	rBV	15298	13521	1.04%	0.105%
37	13.200	1011	1016	1017	rBV3	27048	50043	3.84%	0.390%
38	13.440	1035	1037	1040	rBV	12744	21793	1.67%	0.170%
39	13.554	1044	1047	1048	rBV	24360	37545	2.88%	0.292%
40	13.680	1056	1058	1061	rVB	46955	58564	4.49%	0.456%
41	13.737	1061	1063	1065	rBV2	17914	32836	2.52%	0.256%
42	13.805	1066	1069	1072	rBV2	438277	573790	44.02%	4.467%
43	14.308	1111	1113	1117	rBV3	33841	68624	5.27%	0.534%
44	14.800	1154	1156	1160	rVB	96594	152244	11.68%	1.185%
45	15.063	1177	1179	1182	rVB	63174	85555	6.56%	0.666%
46	15.120	1182	1184	1187	rVV	64970	98425	7.55%	0.766%
47	15.177	1187	1189	1198	rVB	217773	309113	23.72%	2.406%
48	15.611	1225	1227	1230	rBV	36563	70605	5.42%	0.550%

Sum of corrected areas: 12846059

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089056.D
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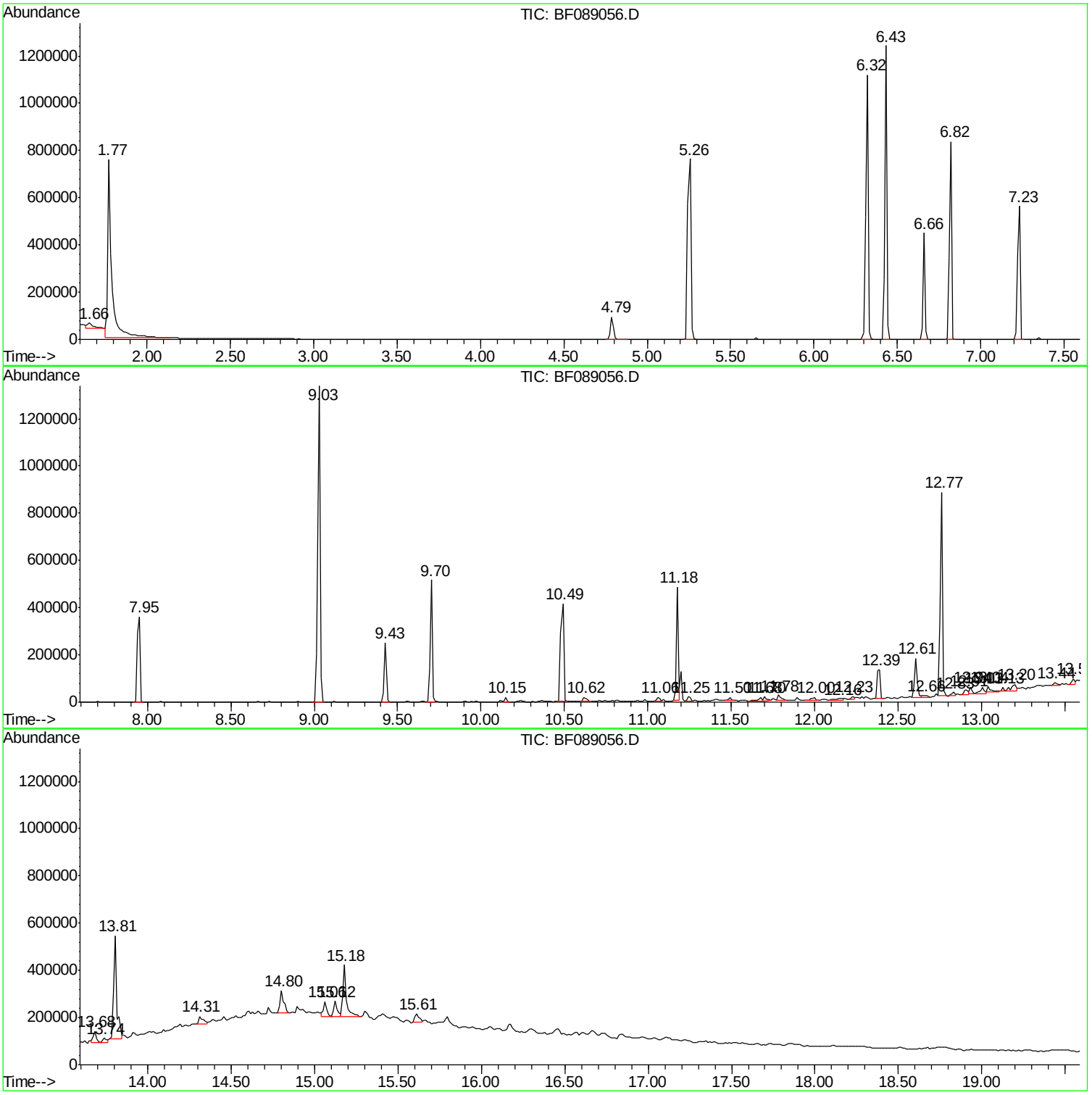
Operator : UM/SJ
Sample : H3989-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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\BF071616\
Data File : BF089056.D
Acq On : 16 Jul 2016 15:40
Operator : UM/SJ
Sample : H3989-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

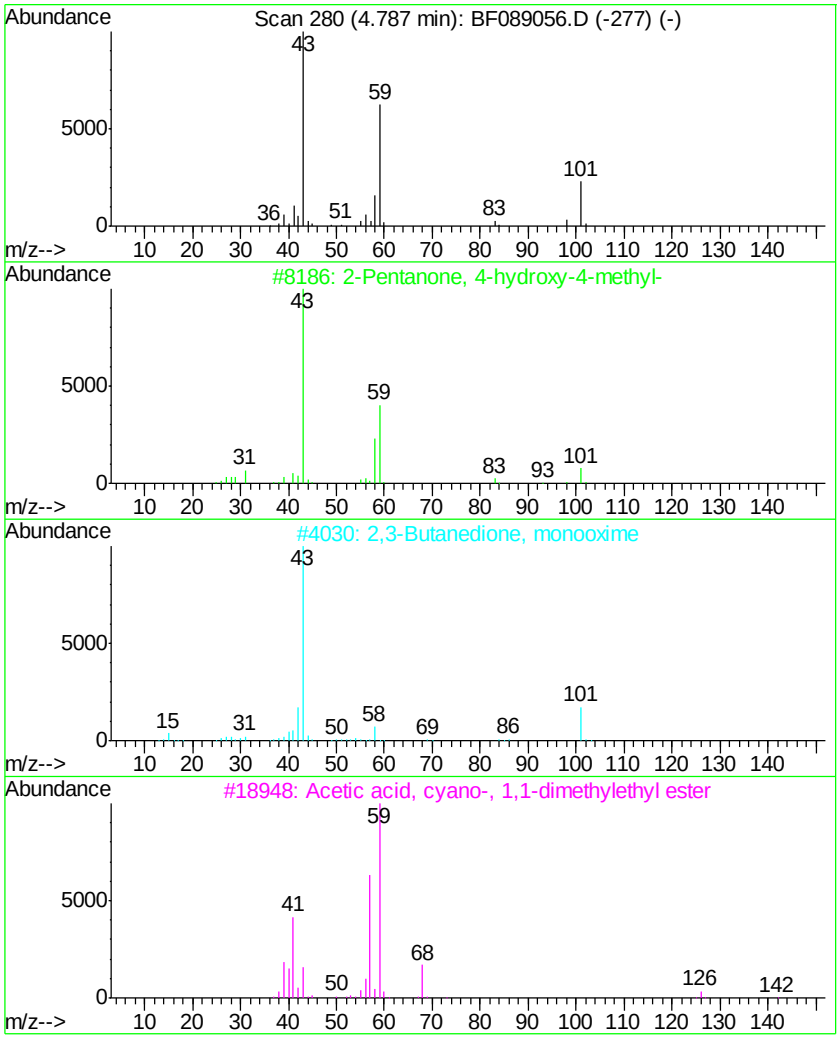
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

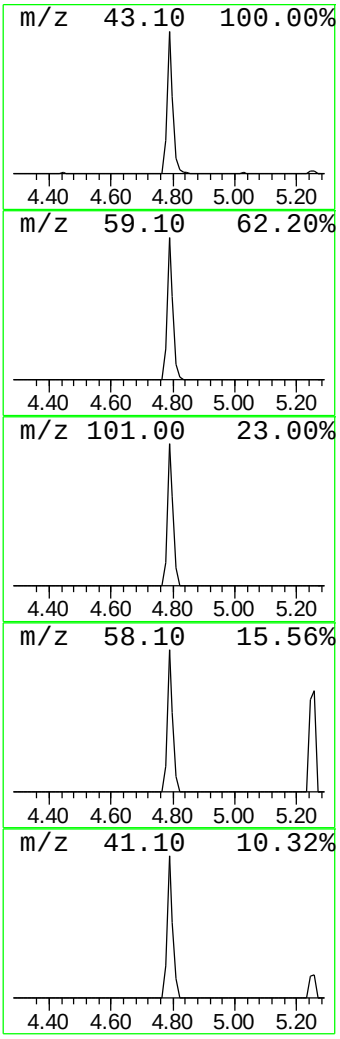
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	6.97 ng	126618	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Acetone	58	C3H6O	000067-64-1	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089056.D
Acq On : 16 Jul 2016 15:40
Operator : UM/SJ
Sample : H3989-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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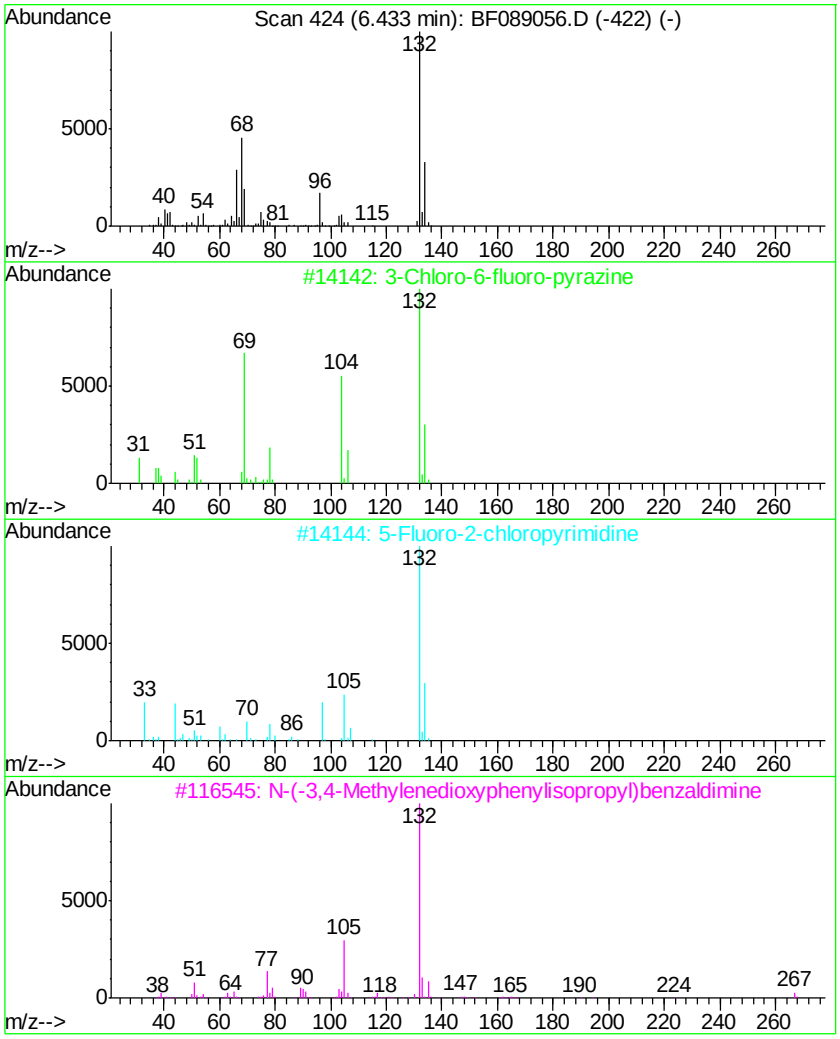
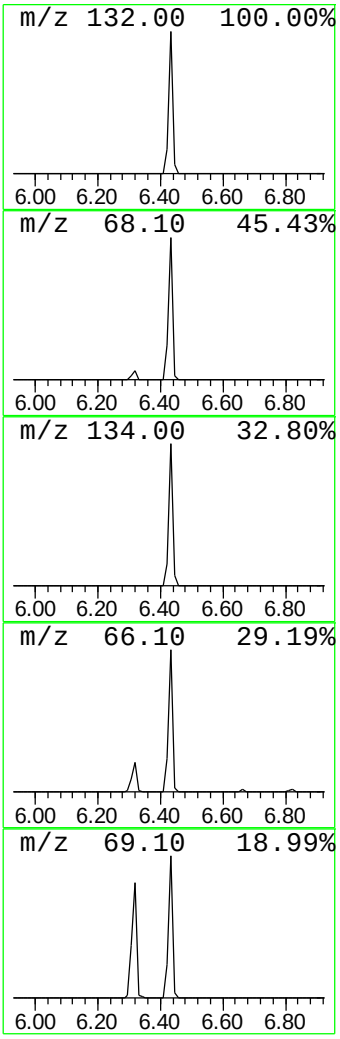
Peak Number 4 unknown6.43 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	58.85 ng	1069300	1,4-Dichlorobenzene-d4	6.66

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	16
3	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089056.D
Acq On : 16 Jul 2016 15:40
Operator : UM/SJ
Sample : H3989-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

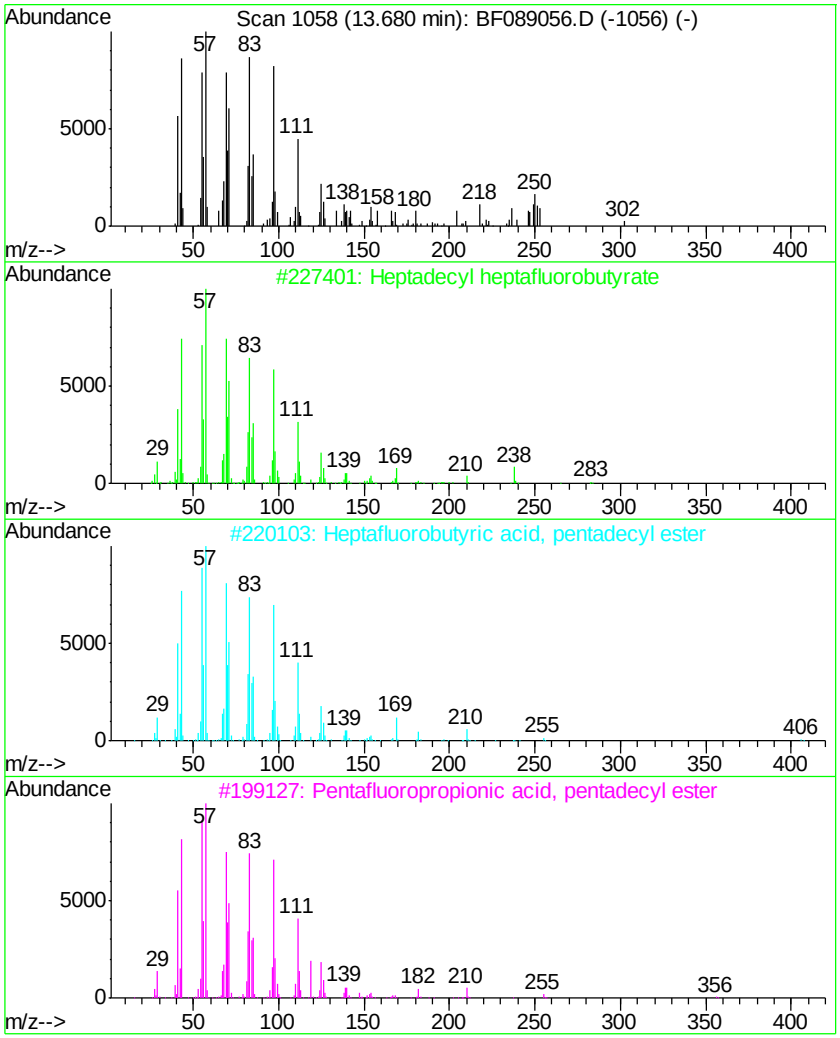
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

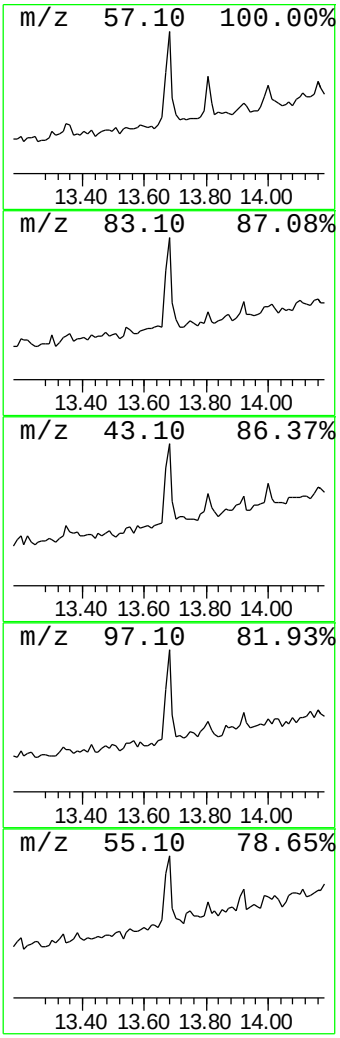
****

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	2.04 ng	58564	Chrysene-d12	13.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	87
5	1-Nonadecene	266	C19H38	018435-45-5	87





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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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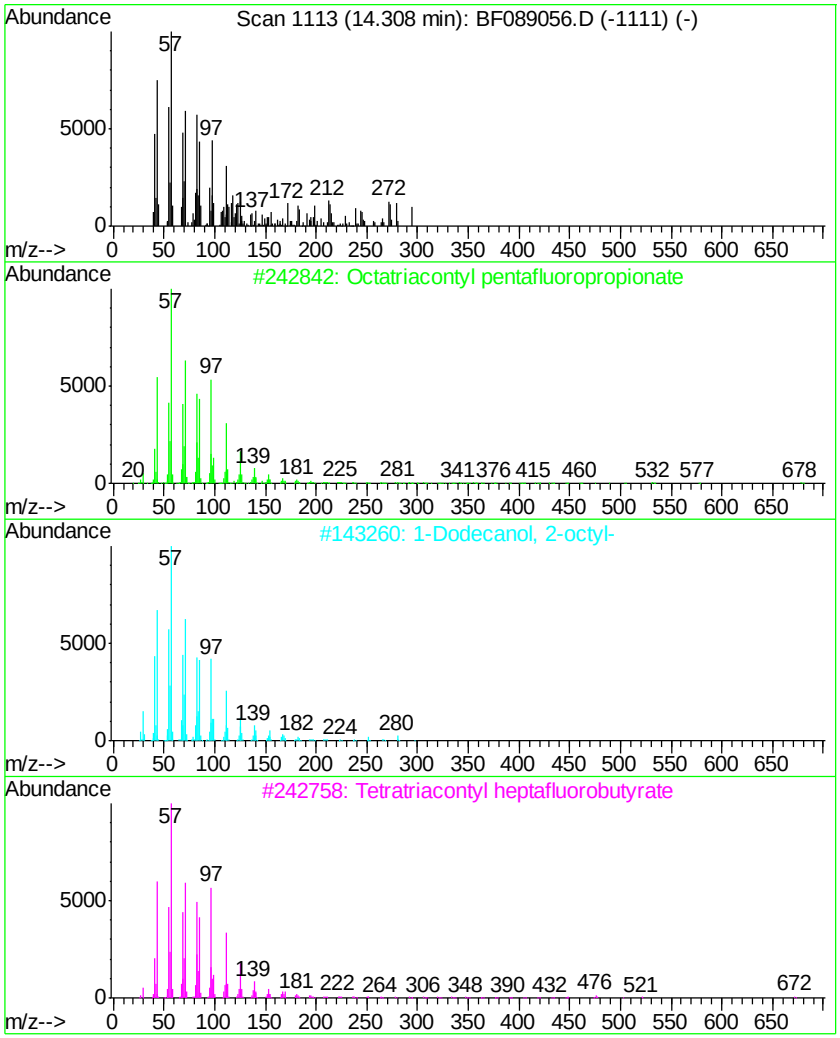
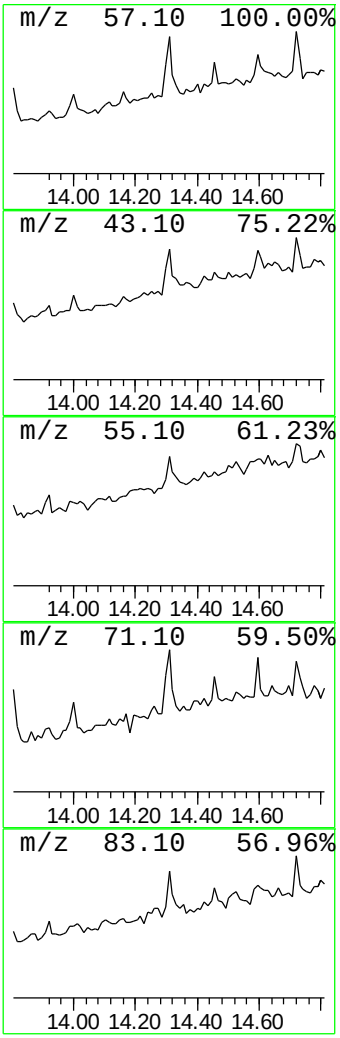
Peak Number 7 Octatriacontyl pentafluorop... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.31	2.39 ng	68624	Chrysene-d12	13.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	50
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	45
3	Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	45
4	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	43
5	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	43





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

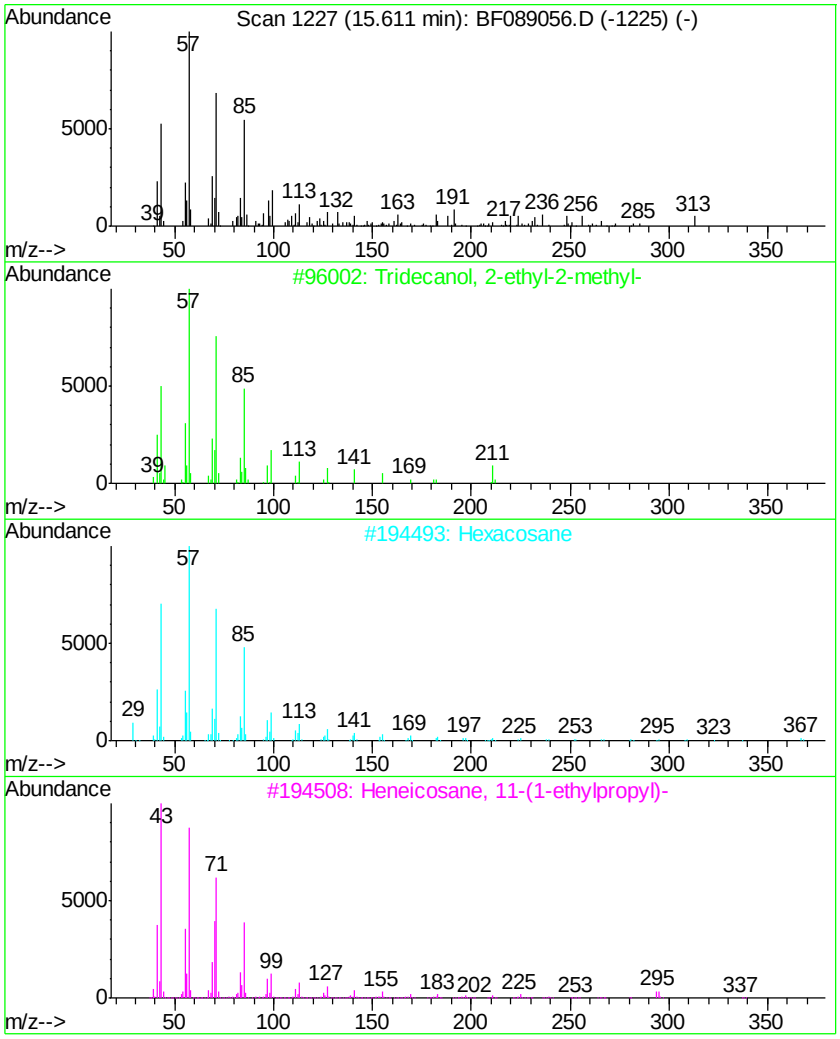
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

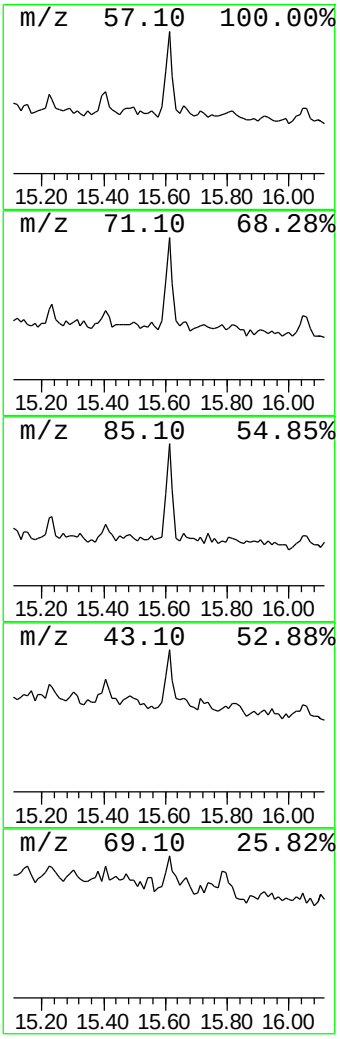
****

Peak Number 9 Tridecanol, 2-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	4.57 ng	70605	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	68
2	Hexacosane	366	C26H54	000630-01-3	68
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	68
4	Heptacosane	380	C27H56	000593-49-7	68
5	Eicosane	282	C20H42	000112-95-8	68





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...	4.79	7.0	ng	126618	1	6.66	363384	20.0
unknown6.43	6.43	58.9	ng	1069300	1	6.66	363384	20.0
Heptadecyl heptaf...	13.68	2.0	ng	58564	5	13.81	573790	20.0
Octatriacontyl pe...	14.31	2.4	ng	68624	5	13.81	573790	20.0
Tridecanol, 2-eth...	15.61	4.6	ng	70605	6	15.18	309113	20.0