LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089067.D
Acq On : 16 Jul 2016 21:13
Operator : UM/SJ
Sample : H4018-16
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E8-B1(0-7)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	1.644	4	5	14	rVB	76570	153223	8.73%	0.979%
2	1.770	14	16	36	rVB	648452	1115800	63.60%	7.131%
3	2.021	36	38	51	rVB2	11959	35075	2.00%	0.224%
4	4.810	280	282	289	rVB	119612	185622	10.58%	1.186%
5	5.267	319	322	324	rBV	1459696	1462103	83.33%	9.344%
6	6.330	411	415	417	rBV	1404664	1530135	87.21%	9.779%
7	6.444	422	425	427	rBV	1657977	1670033	95.18%	10.673%
8	6.662	442	444	446	rBV	299185	350796	19.99%	2.242%
9	6.822	456	458	461	rVB	1206840	1117901	63.72%	7.144%
10	7.233	491	494	497	rBV	787058	801224	45.67%	5.121%
11	7.953	555	557	559	rBV	632013	500312	28.52%	3.197%
12	9.039	649	652	654	rBV	1473349	1754528	100.00%	11.213%
13	9.428	684	686	689	rBV	287462	256475	14.62%	1.639%
14	9.702	708	710	712	rBV	506358	449073	25.60%	2.870%
15	10.148	748	749	751	rVB	17023	18501	1.05%	0.118%
16	10.490	777	779	782	rBV	664776	651298	37.12%	4.162%
17	10.628	789	791	795	rBV	24319	40059	2.28%	0.256%
18	11.073	828	830	831	rBV	25273	26690	1.52%	0.171%
19	11.188	837	840	843	rVV	307241	412511	23.51%	2.636%
20	11.256	843	846	848	rVB	30747	29050	1.66%	0.186%
21	11.428	858	861	864	rBV2	14363	20282	1.16%	0.130%
22	11.793	891	893	898	rVB	29234	39056	2.23%	0.250%
23	11.999	907	911	915	rBV	13433	25371	1.45%	0.162%
24	12.228	930	931	933	rBV	11707	19157	1.09%	0.122%
25	12.388	943	945	947	rBV	167862	150102	8.56%	0.959%
26	12.536	955	958	960	rBV3	8408	18089	1.03%	0.116%
27	12.616	962	965	967	rVV	163358	169991	9.69%	1.086%
28	12.662	967	969	973	rVB3	12979	22067	1.26%	0.141%
29	12.776	976	979	981	rVB	911224	1118076	63.73%	7.146%
30	12.845	981	985	988	rBV3	11963	28849	1.64%	0.184%
31	12.948	990	994	996	rVV	22422	35608	2.03%	0.228%
32	13.051	1001	1003	1004	rBV	23881	23430	1.34%	0.150%
33	13.176	1012	1014	1016	rBV3	13177	22416	1.28%	0.143%
34	13.451	1037	1038	1041	rBV2	17169	28176	1.61%	0.180%

LSC Area Percent Report

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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E8-B1(0-7)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

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Peak separation: 5

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

35	13.554	1045	1047	1049	rBV2	19504	37238	2.12%	0.238%
36	13.679	1056	1058	1061	rVB2	63664	71894	4.10%	0.459%
37	13.817	1066	1070	1071	rBV2	388646	564217	32.16%	3.606%
38	14.731	1148	1150	1152	rBV	83808	87343	4.98%	0.558%
39	14.811	1155	1157	1161	rVB	71371	131795	7.51%	0.842%
40	14.902	1163	1165	1170	rBV2	68275	113615	6.48%	0.726%
41	15.131	1183	1185	1188	rBV	47360	61601	3.51%	0.394%
42	15.188	1188	1190	1193	rBV	190009	230267	13.12%	1.472%
43	15.622	1226	1228	1231	rBV	47306	68125	3.88%	0.435%

Sum of corrected areas: 15647174

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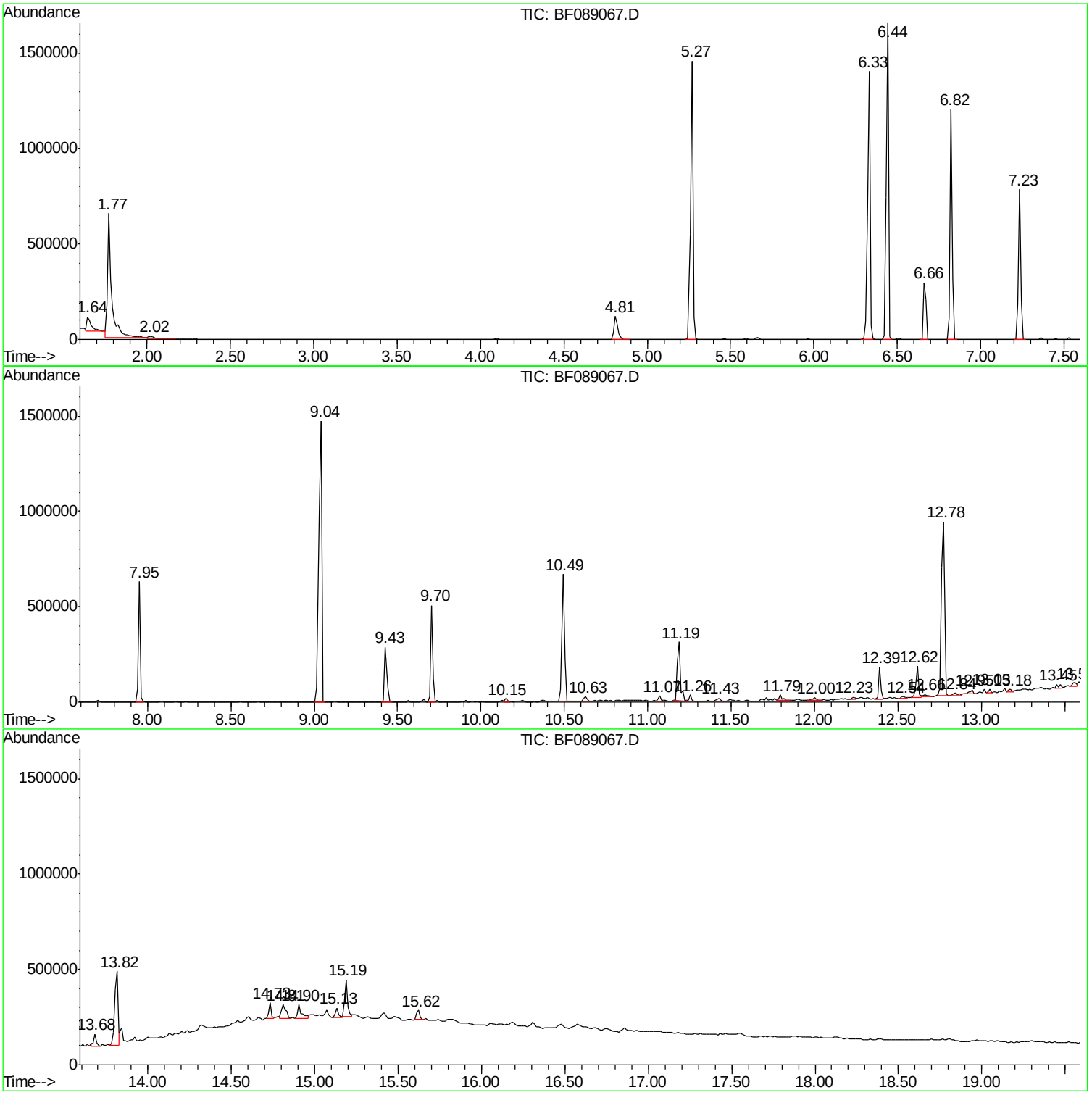
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E8-B1(0-7)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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Data File : BF089067.D
Acq On : 16 Jul 2016 21:13
Operator : UM/SJ
Sample : H4018-16
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E8-B1(0-7)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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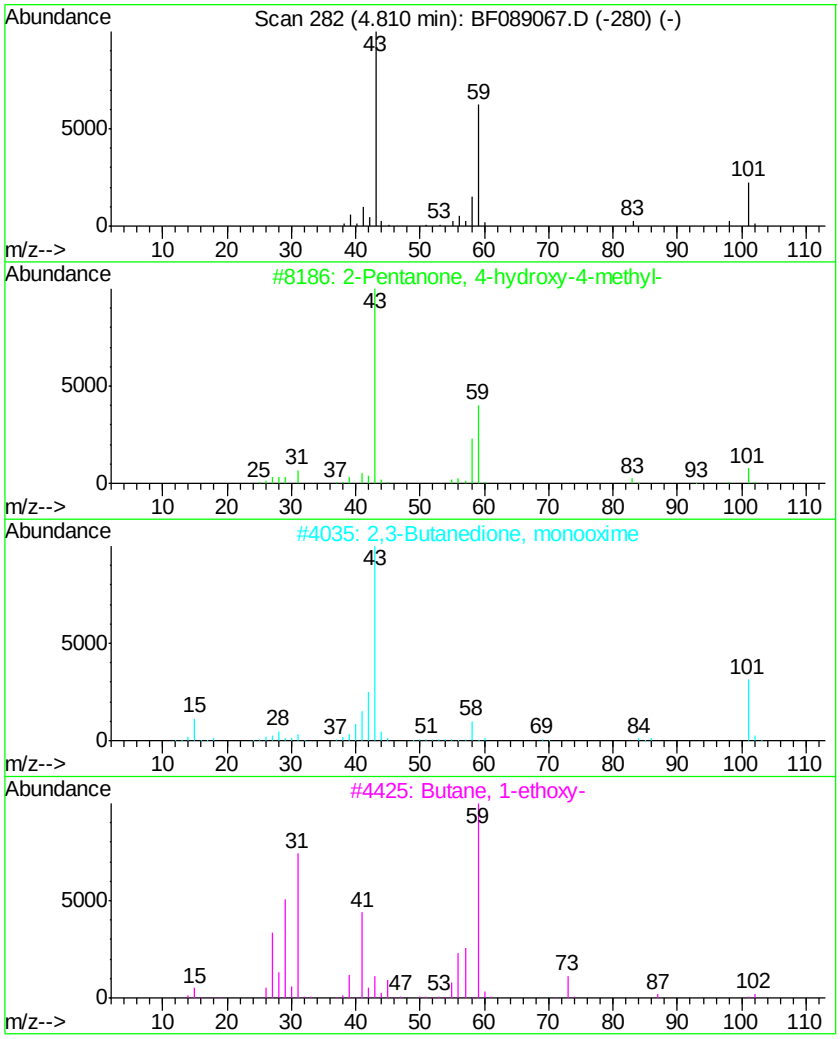
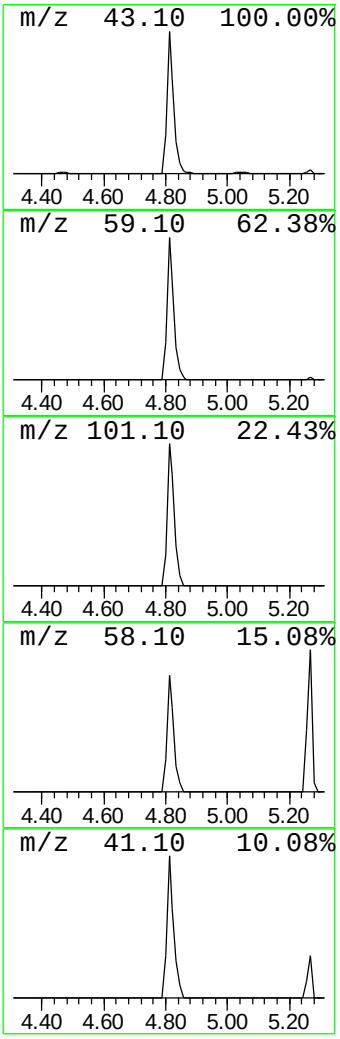
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	10.58 ng	185622	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	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Data File : BF089067.D
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Operator : UM/SJ
Sample : H4018-16
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E8-B1(0-7)C

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

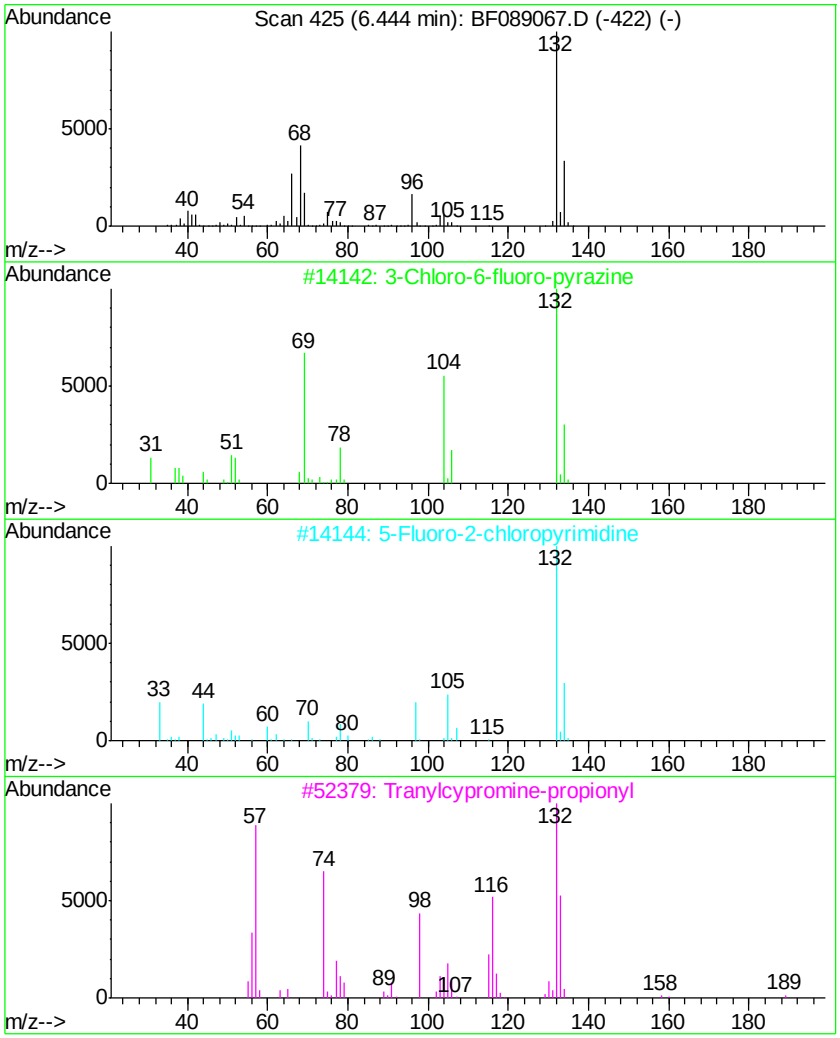
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

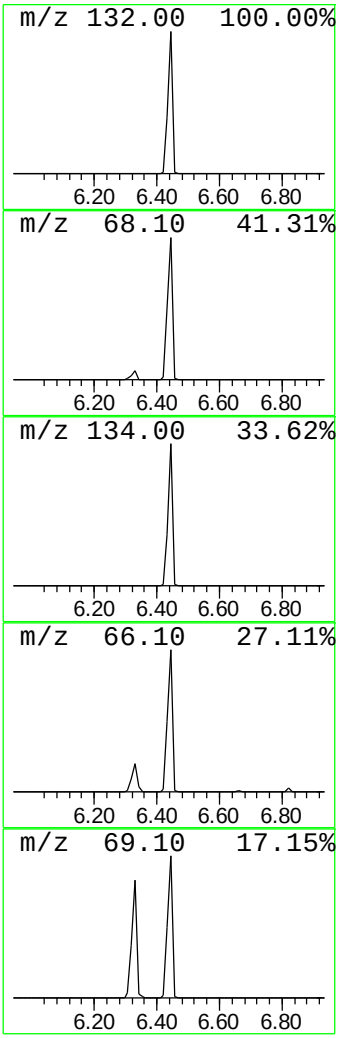
****

Peak Number 4 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	95.21 ng	1670030	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	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
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Instrument : BNA_F
ClientSampleId : E8-B1(0-7)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
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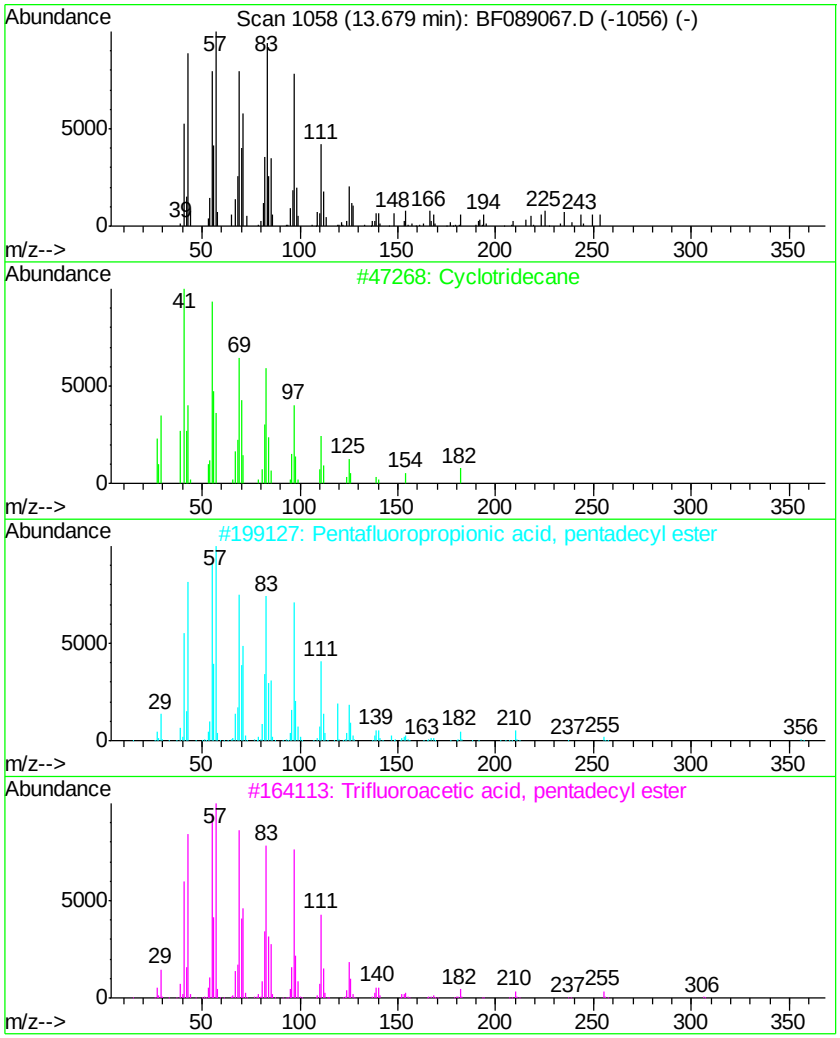
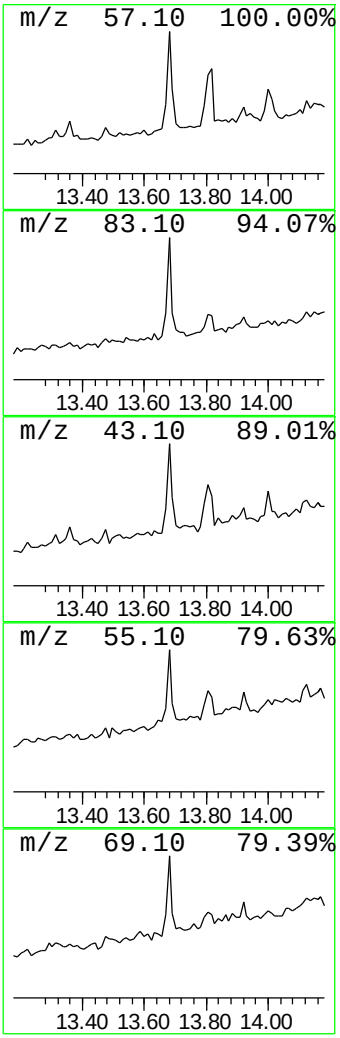
Peak Number 6 Cyclotridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	2.55 ng	71894	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotridecane	182	C13H26	000295-02-3	95
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : E8-B1(0-7)C

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TIC Library : C:\Database\NIST11.L
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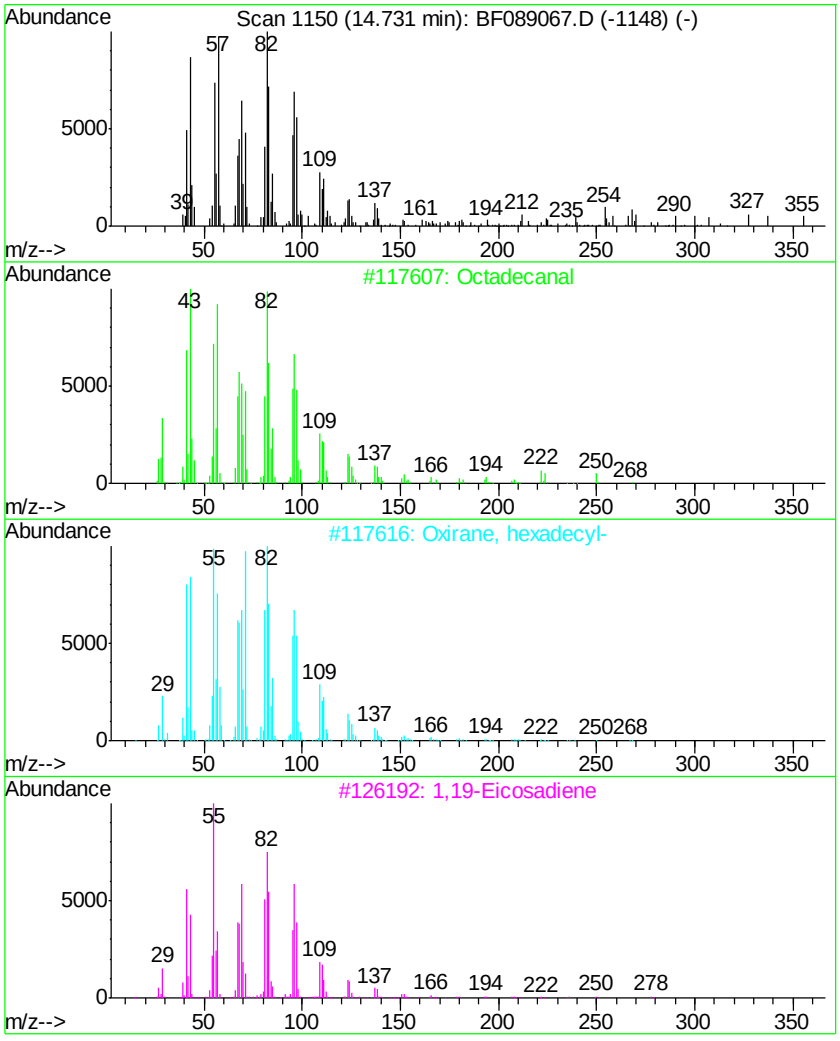
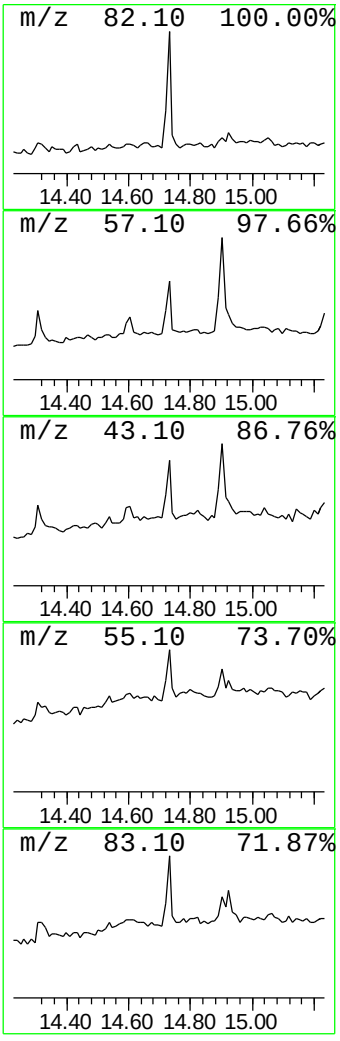
Peak Number 7 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	7.59 ng	87343	Perylene-d12	15.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	90
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
3	1,19-Eicosadiene	278	C20H38	014811-95-1	87
4	18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	72
5	1,13-Tetradecadiene	194	C14H26	021964-49-8	68





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Operator : UM/SJ
Sample : H4018-16
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : E8-B1(0-7)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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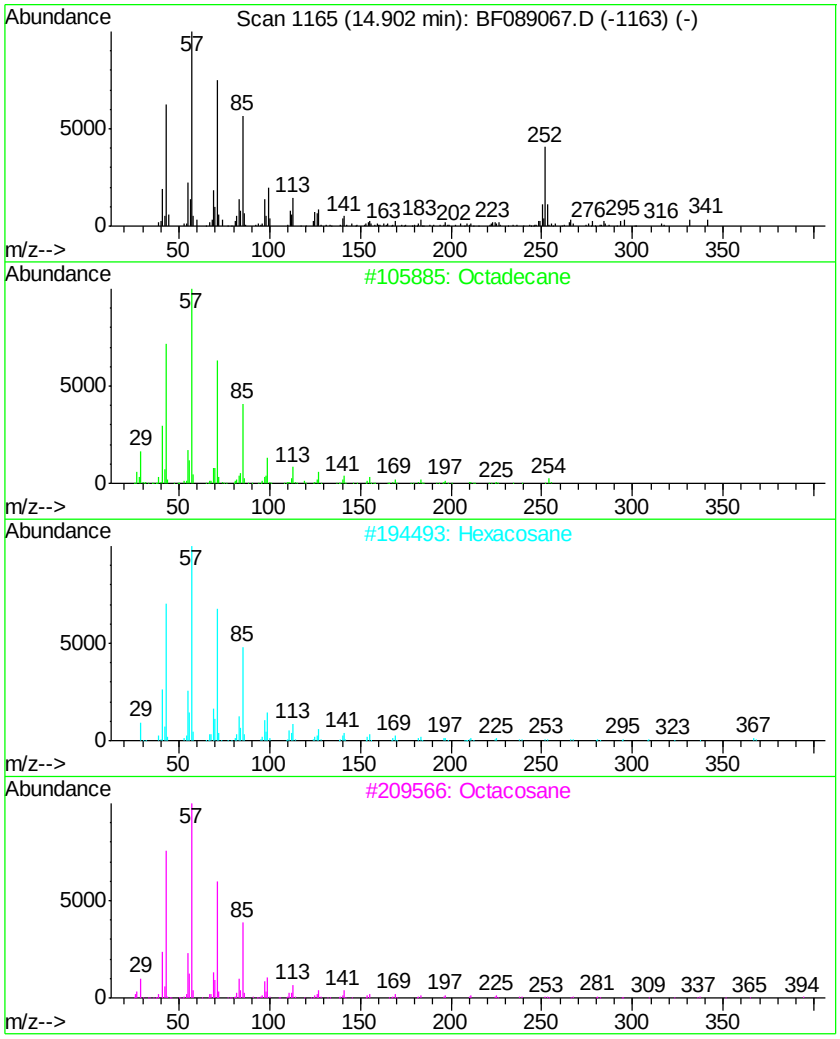
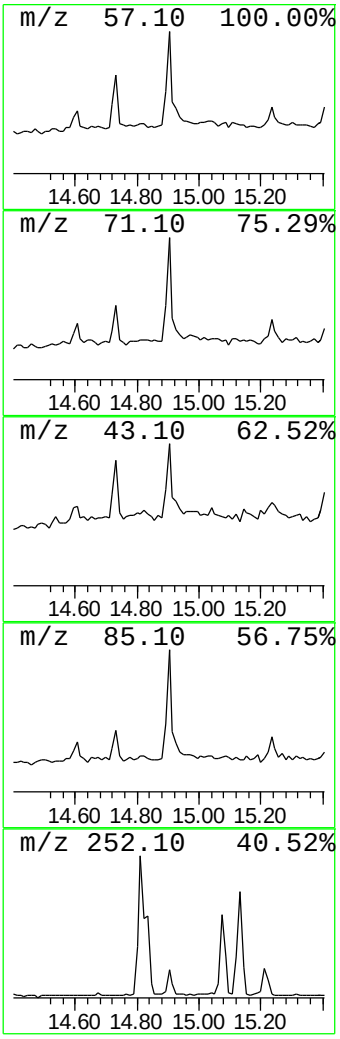
Peak Number 8 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	9.87 ng	113615	Perylene-d12	15.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	83
2	Hexacosane	366	C26H54	000630-01-3	70
3	Octacosane	394	C28H58	000630-02-4	64
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	62
5	Heptadecane	240	C17H36	000629-78-7	62





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Instrument : BNA_F
ClientSampleId : E8-B1(0-7)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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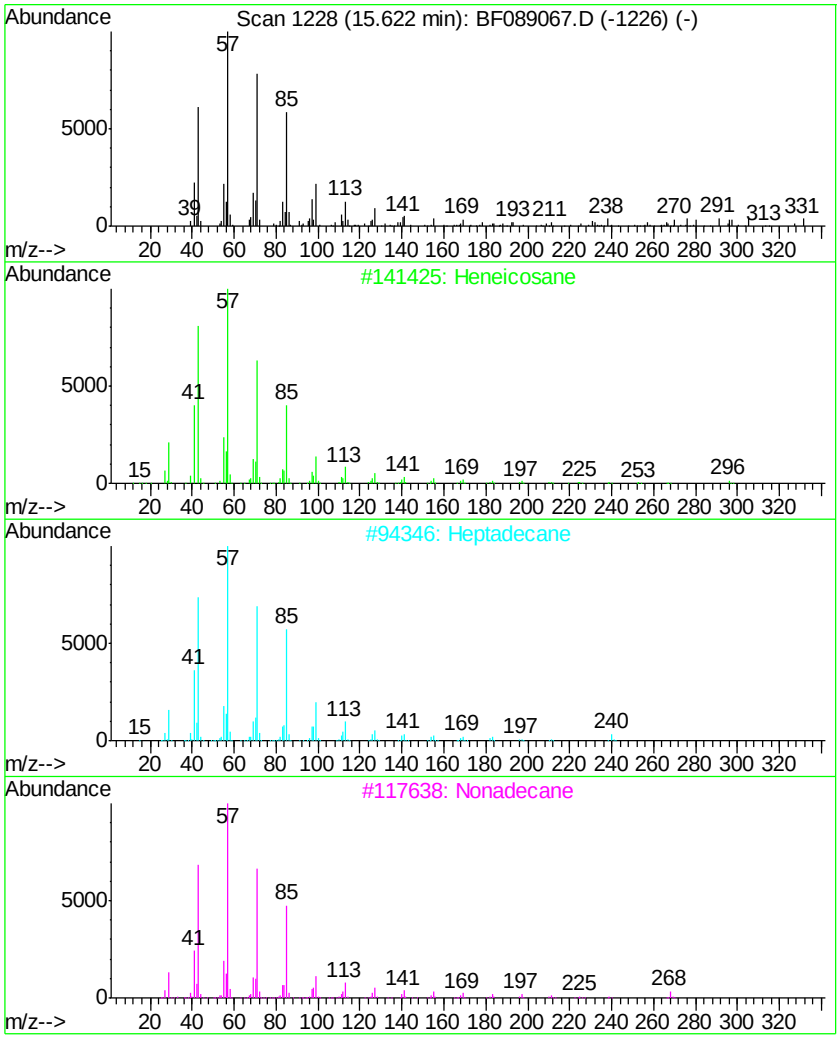
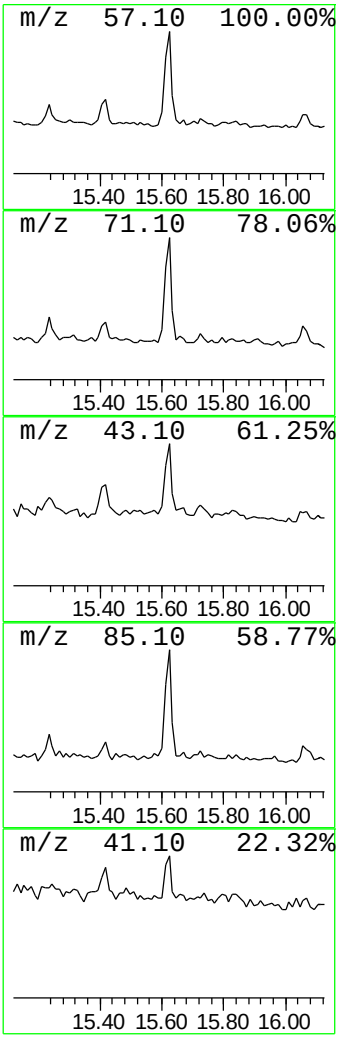
Peak Number 9 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	5.92 ng	68125	Perylene-d12	15.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	81
2	Heptadecane	240	C17H36	000629-78-7	81
3	Nonadecane	268	C19H40	000629-92-5	76
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	74
5	Hexacosane	366	C26H54	000630-01-3	72





Tentatively Identified Compound (LSC) summary

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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.81	10.6	ng	185622	1	6.66	350796	20.0
unknown6.44	6.44	95.2	ng	1670030	1	6.66	350796	20.0
Cyclotridecane	13.68	2.5	ng	71894	5	13.82	564217	20.0
Octadecanal	14.73	7.6	ng	87343	6	15.19	230267	20.0
Octadecane	14.90	9.9	ng	113615	6	15.19	230267	20.0
Heneicosane	15.62	5.9	ng	68125	6	15.19	230267	20.0