LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089058.D
Acq On : 16 Jul 2016 16:41
Operator : UM/SJ
Sample : H3989-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B3(0-6)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	67223	138750	9.20%	1.024%
2	1.770	14	16	53	rVB	784414	1507805	100.00%	11.131%
3	2.776	102	104	114	rBV	6027	17305	1.15%	0.128%
4	4.799	279	281	286	rBB	102344	139202	9.23%	1.028%
5	5.256	319	321	324	rBV	1215501	1162888	77.12%	8.585%
6	6.319	411	414	416	rBV	1212194	1244147	82.51%	9.185%
7	6.433	422	424	426	rBV	1397316	1219261	80.86%	9.001%
8	6.662	442	444	446	rBB	468302	371637	24.65%	2.743%
9	6.822	455	458	460	rBB	1198368	1075727	71.34%	7.941%
10	7.233	491	494	496	rBV	810076	825042	54.72%	6.091%
11	7.530	518	520	524	rVB	48751	53591	3.55%	0.396%
12	7.953	554	557	559	rBV	405121	459924	30.50%	3.395%
13	8.170	574	576	578	rBV	39229	30341	2.01%	0.224%
14	8.228	579	581	583	rBB	49808	37612	2.49%	0.278%
15	9.028	648	651	653	rVB	1524583	1340891	88.93%	9.899%
16	9.428	684	686	688	rBV	280940	225597	14.96%	1.665%
17	9.702	707	710	712	rBV	546196	464487	30.81%	3.429%
18	10.148	748	749	751	rVB	25272	19681	1.31%	0.145%
19	10.365	766	768	771	rBV	12689	19390	1.29%	0.143%
20	10.491	777	779	781	rVB	571190	583102	38.67%	4.305%
21	10.628	789	791	794	rBV	25397	50665	3.36%	0.374%
22	11.062	827	829	831	rBV	19730	29548	1.96%	0.218%
23	11.176	837	839	843	rVB	437248	384146	25.48%	2.836%
24	11.496	864	867	869	rBV	24280	27241	1.81%	0.201%
25	11.782	891	892	898	rVB2	11643	17758	1.18%	0.131%
26	12.388	943	945	947	rBV	49989	57384	3.81%	0.424%
27	12.434	947	949	951	rBV3	12369	15362	1.02%	0.113%
28	12.548	956	959	960	rBV3	12204	26508	1.76%	0.196%
29	12.605	962	964	968	rBV	57307	90783	6.02%	0.670%
30	12.765	976	978	981	rBV	1090224	1004925	66.65%	7.419%
31	12.937	991	993	995	rBV3	18088	27925	1.85%	0.206%
32	13.131	1008	1010	1012	rBV2	17923	24267	1.61%	0.179%
33	13.200	1014	1016	1018	rVV3	24058	36260	2.40%	0.268%
34	13.680	1056	1058	1061	rBV2	56952	67230	4.46%	0.496%

LSC Area Percent Report

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Operator : UM/SJ
Sample : H3989-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.805	1067	1069	1073	rBV	371859	427585	28.36%	3.157%
36	15.177	1187	1189	1199	rVB	153269	322139	21.36%	2.378%

Sum of corrected areas: 13546106

LSC Report - Integrated Chromatogram

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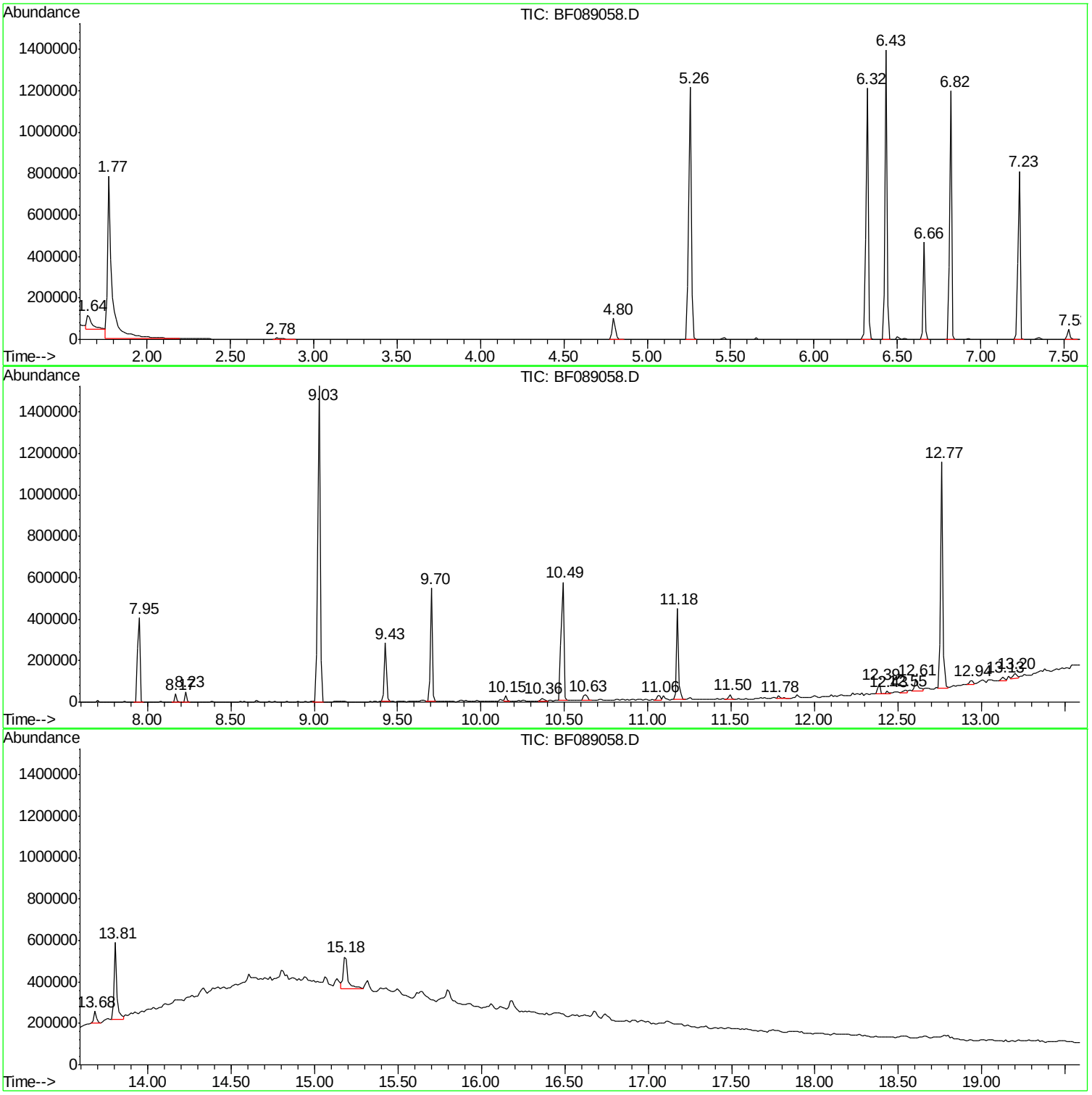
Acq On : 16 Jul 2016 16:41
Operator : UM/SJ
Sample : H3989-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B3(0-6)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 : BF089058.D
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Operator : UM/SJ
Sample : H3989-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B3(0-6)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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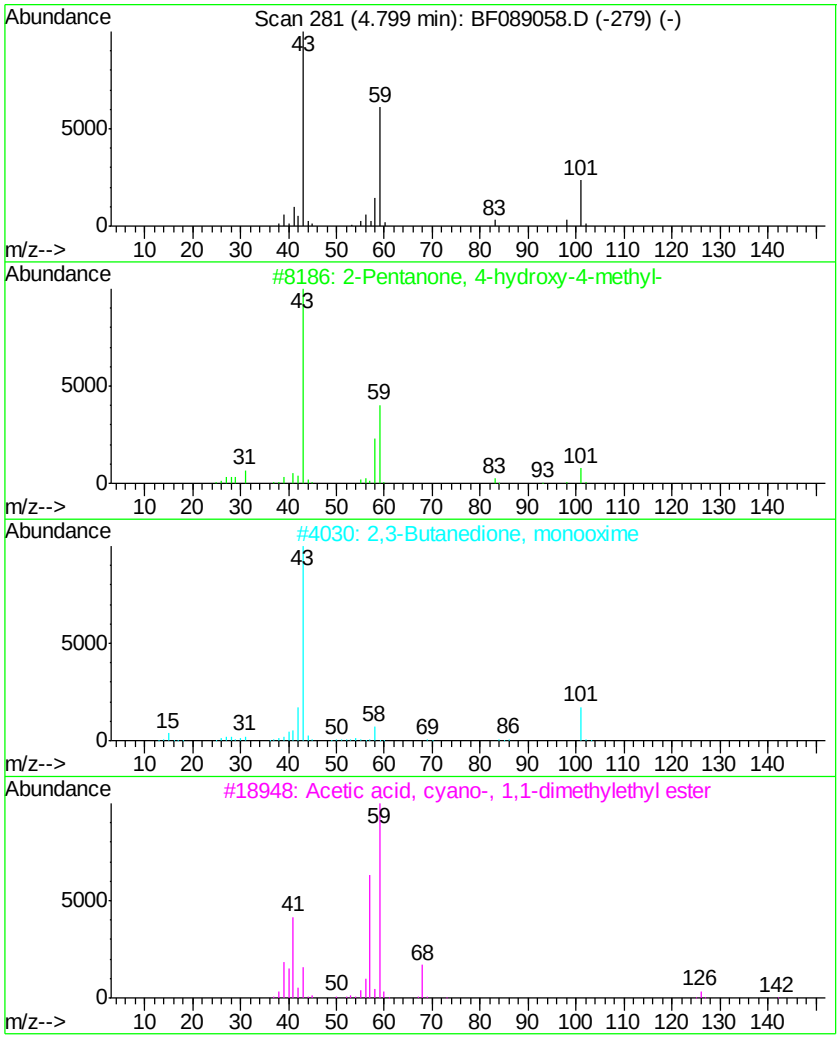
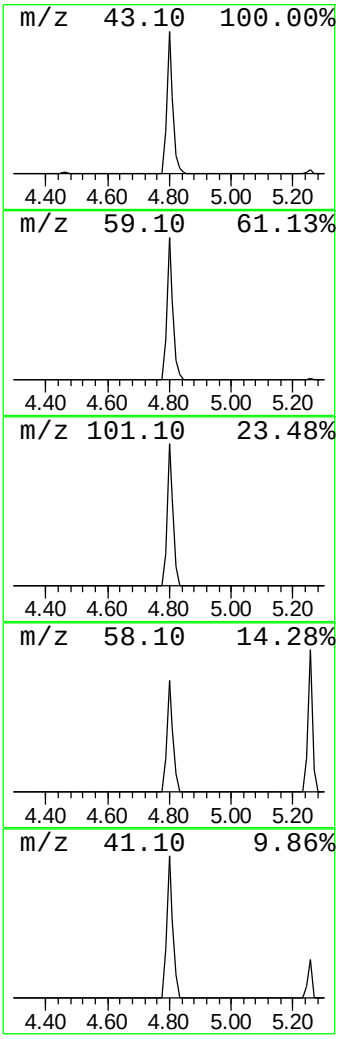
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	7.49 ng	139202	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	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089058.D
Acq On : 16 Jul 2016 16:41
Operator : UM/SJ
Sample : H3989-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B3(0-6)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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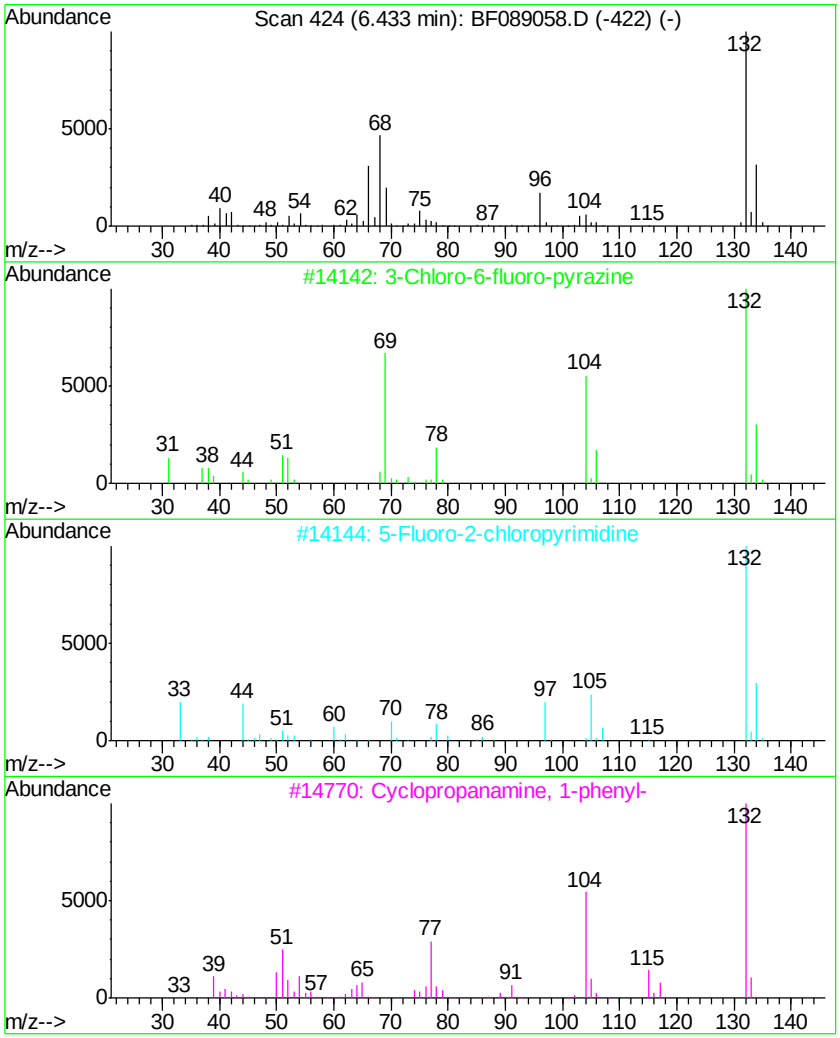
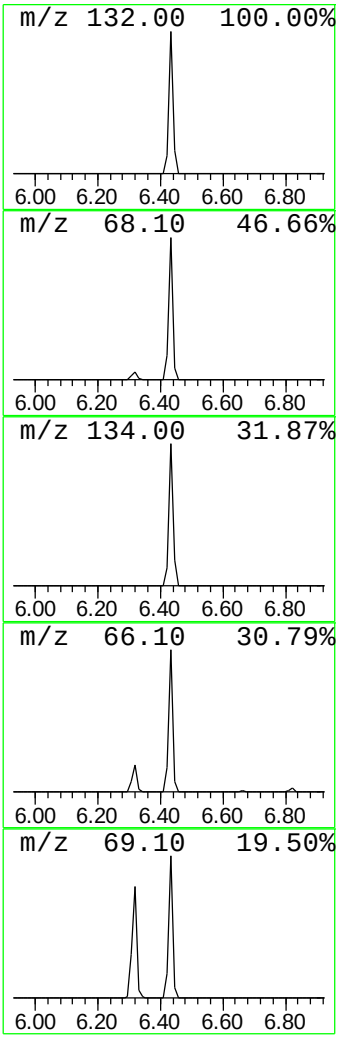
Peak Number 4 unknown6.43 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	65.62 ng	1219260	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	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





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Sample : H3989-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B3(0-6)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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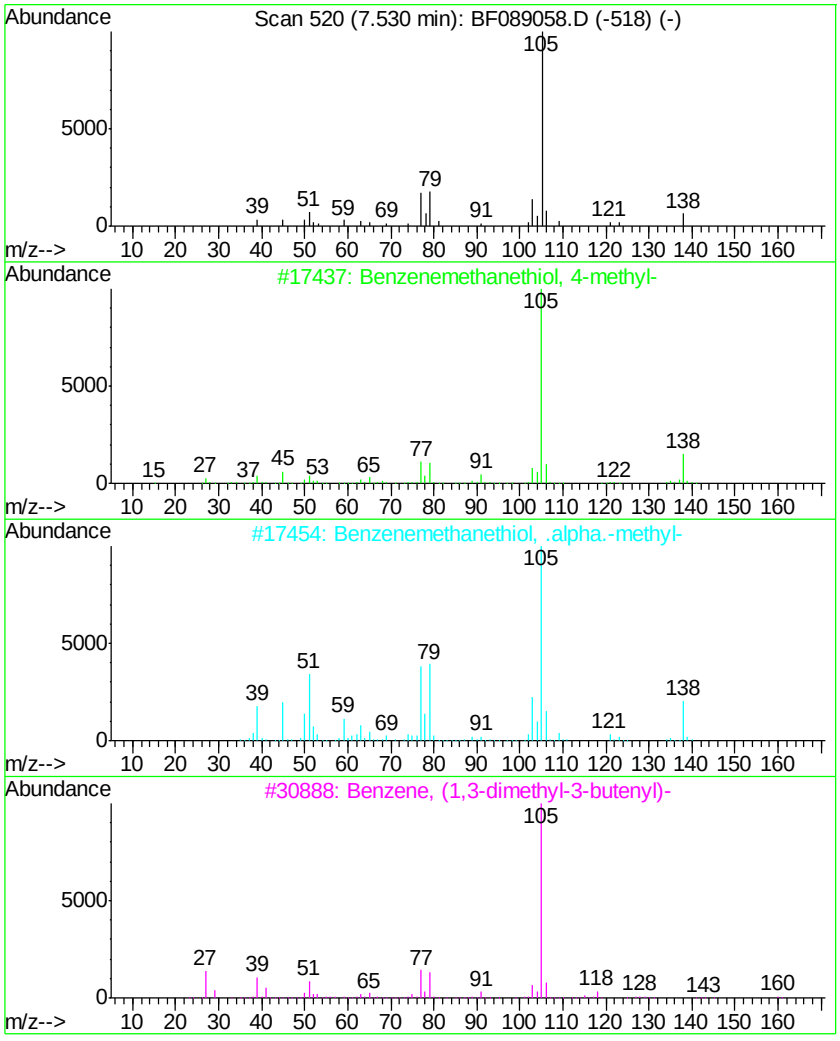
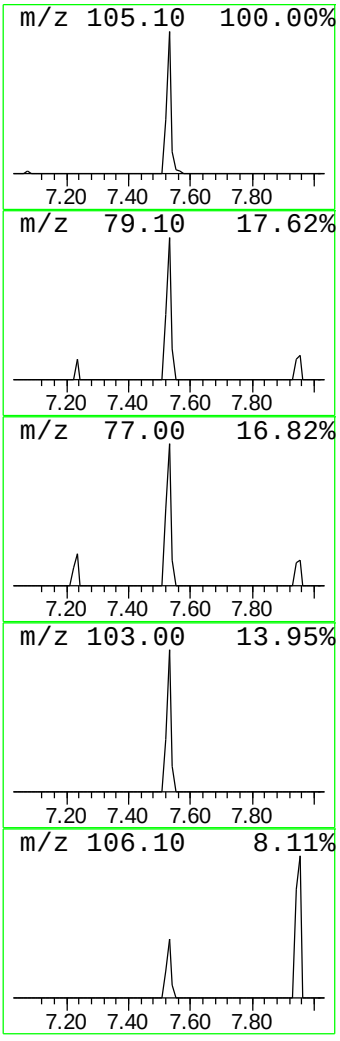
Peak Number 6 Benzenemethanethiol, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	2.33 ng	53591	Naphthalene-d8	7.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenemethanethiol, 4-methyl-	138	C8H10S	004498-99-1	78
2	Benzenemethanethiol, .alpha.-met...	138	C8H10S	006263-65-6	74
3	Benzene, (1,3-dimethyl-3-butenyl)-	160	C12H16	056851-51-5	64
4	Ether, p-methylbenzyl vinyl	148	C10H12O	026437-10-5	64
5	Benzene, 1-(bromomethyl)-4-methyl-	184	C8H9Br	000104-81-4	64





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Operator : UM/SJ
Sample : H3989-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : Q7-B3(0-6)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
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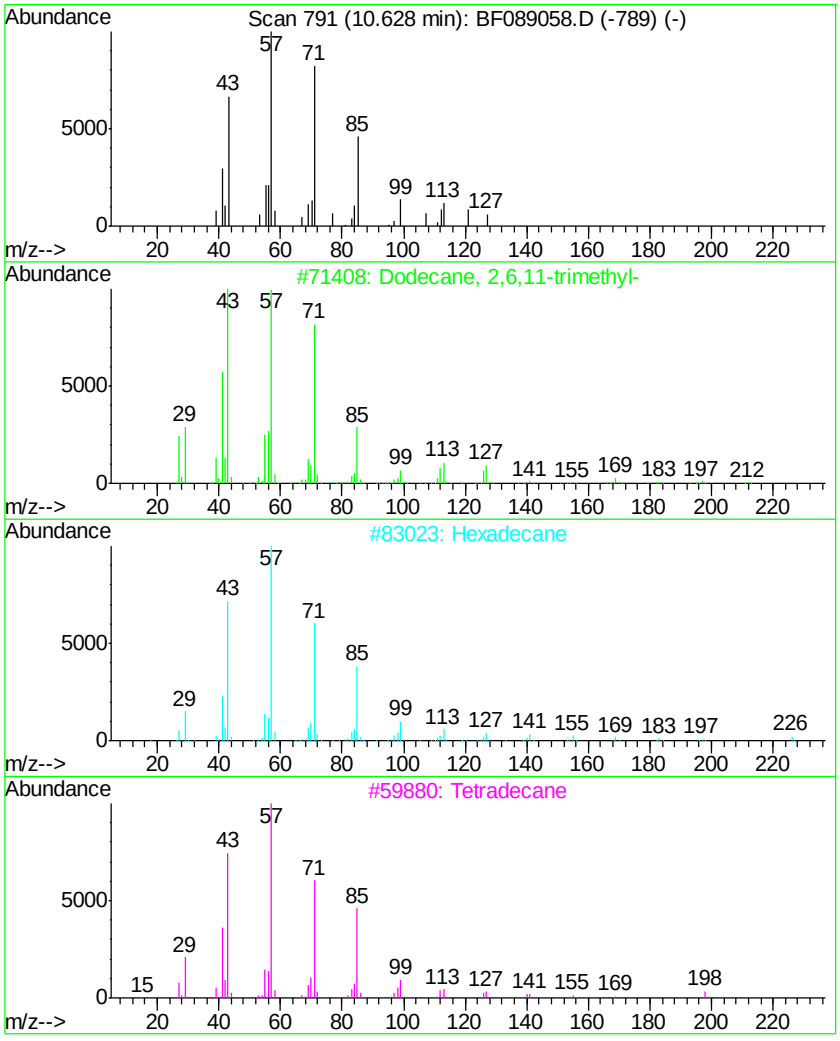
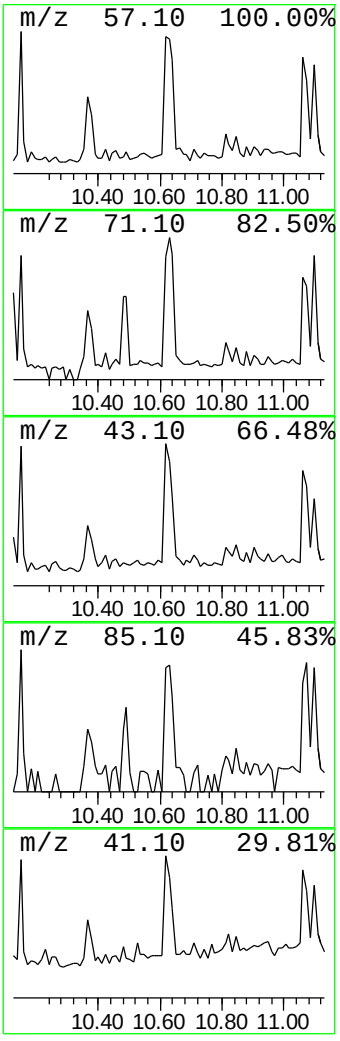
****

Peak Number 7 Dodecane, 2,6,11-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	2.64 ng	50665	Phenanthrene-d10	11.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	80
2	Hexadecane	226	C16H34	000544-76-3	78
3	Tetradecane	198	C14H30	000629-59-4	78
4	Tridecane	184	C13H28	000629-50-5	78
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
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Instrument : BNA_F
ClientSampleId : Q7-B3(0-6)C

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

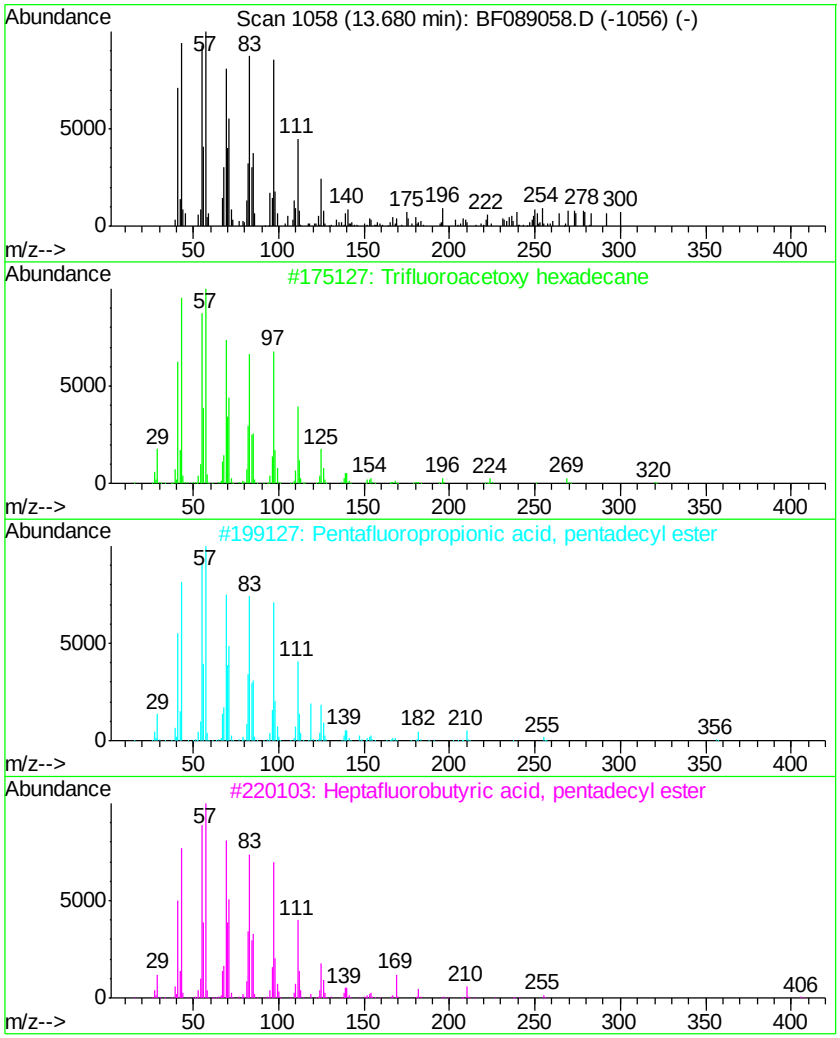
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

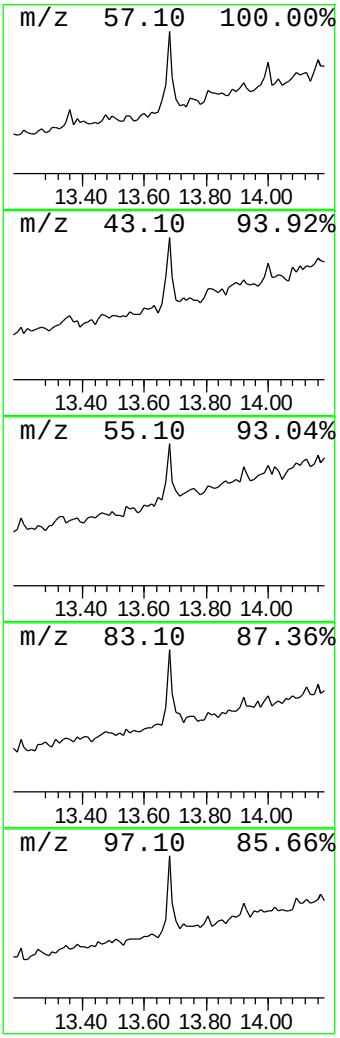
****

Peak Number 9 Trifluoroacetoxy hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	3.14 ng	67230	Chrysene-d12	13.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	7.5	ng	139202	1	6.66	371637	20.0
unknown6.43	6.43	65.6	ng	1219260	1	6.66	371637	20.0
Benzenemethanethi...	7.53	2.3	ng	53591	2	7.95	459924	20.0
Dodecane, 2,6,11-...	10.63	2.6	ng	50665	4	11.18	384146	20.0
Trifluoroacetoxy ...	13.68	3.1	ng	67230	5	13.81	427585	20.0