LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101017\
Data File : BF099319.D
Acq On : 11 Oct 2017 00:12
Operator : SJ/JU
Sample : I5691-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-115-8(5-10)

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-BF092317.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	5.075	505	508	519	rBV	216851	248498	13.91%	1.509%
2	5.481	573	577	588	rBV	1688694	1565244	87.62%	9.503%
3	6.492	745	749	765	rBV	1557248	1603046	89.74%	9.732%
4	6.634	769	773	776	rBV	1969142	1646082	92.15%	9.994%
5	6.863	808	812	816	rBV	678763	525472	29.42%	3.190%
6	7.022	834	839	842	rBV	1408999	1276426	71.45%	7.749%
7	7.428	903	908	911	rBV	1113051	949891	53.17%	5.767%
8	8.145	1026	1030	1033	rBV	830888	643608	36.03%	3.907%
9	8.792	1132	1140	1142	rBV4	13446	20748	1.16%	0.126%
10	9.016	1174	1178	1182	rBV4	16354	26595	1.49%	0.161%
11	9.145	1193	1200	1203	rBV7	14572	38021	2.13%	0.231%
12	9.216	1208	1212	1218	rBV	1908039	1786387	100.00%	10.846%
13	9.292	1220	1225	1228	rVB5	27522	44904	2.51%	0.273%
14	9.410	1243	1245	1248	rBV4	21623	21728	1.22%	0.132%
15	9.610	1276	1279	1286	rBV	295086	264475	14.81%	1.606%
16	9.898	1325	1328	1332	rVB	696185	594423	33.28%	3.609%
17	10.692	1459	1463	1467	rBV	713755	743150	41.60%	4.512%
18	11.386	1578	1581	1584	rBV	539014	488986	27.37%	2.969%
19	12.968	1847	1850	1854	rVB	1366635	1266973	70.92%	7.692%
20	13.186	1885	1887	1890	rVB	86006	72323	4.05%	0.439%
21	13.527	1942	1945	1948	rVB	148422	128940	7.22%	0.783%
22	13.857	1998	2001	2014	rVB	271867	289161	16.19%	1.756%
23	13.992	2021	2024	2027	rVB	100385	75433	4.22%	0.458%
24	14.027	2027	2030	2034	rBV	584747	513713	28.76%	3.119%
25	14.168	2051	2054	2059	rVB	217023	201371	11.27%	1.223%
26	14.474	2103	2106	2109	rVB	273656	219221	12.27%	1.331%
27	14.639	2132	2134	2136	rVB	33881	24536	1.37%	0.149%
28	14.780	2155	2158	2164	rVB	214283	209214	11.71%	1.270%
29	15.115	2212	2215	2220	rVB	177494	194283	10.88%	1.180%
30	15.504	2276	2281	2288	rVB2	414294	564689	31.61%	3.428%
31	15.927	2349	2353	2360	rVB	73188	111286	6.23%	0.676%
32	16.433	2436	2439	2445	rVB2	40176	62920	3.52%	0.382%
33	17.021	2537	2539	2546	rVB5	30616	49395	2.77%	0.300%

LSC Area Percent Report

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Data File : BF099319.D
Acq On : 11 Oct 2017 00:12
Operator : SJ/JU
Sample : I5691-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-115-8(5-10)

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

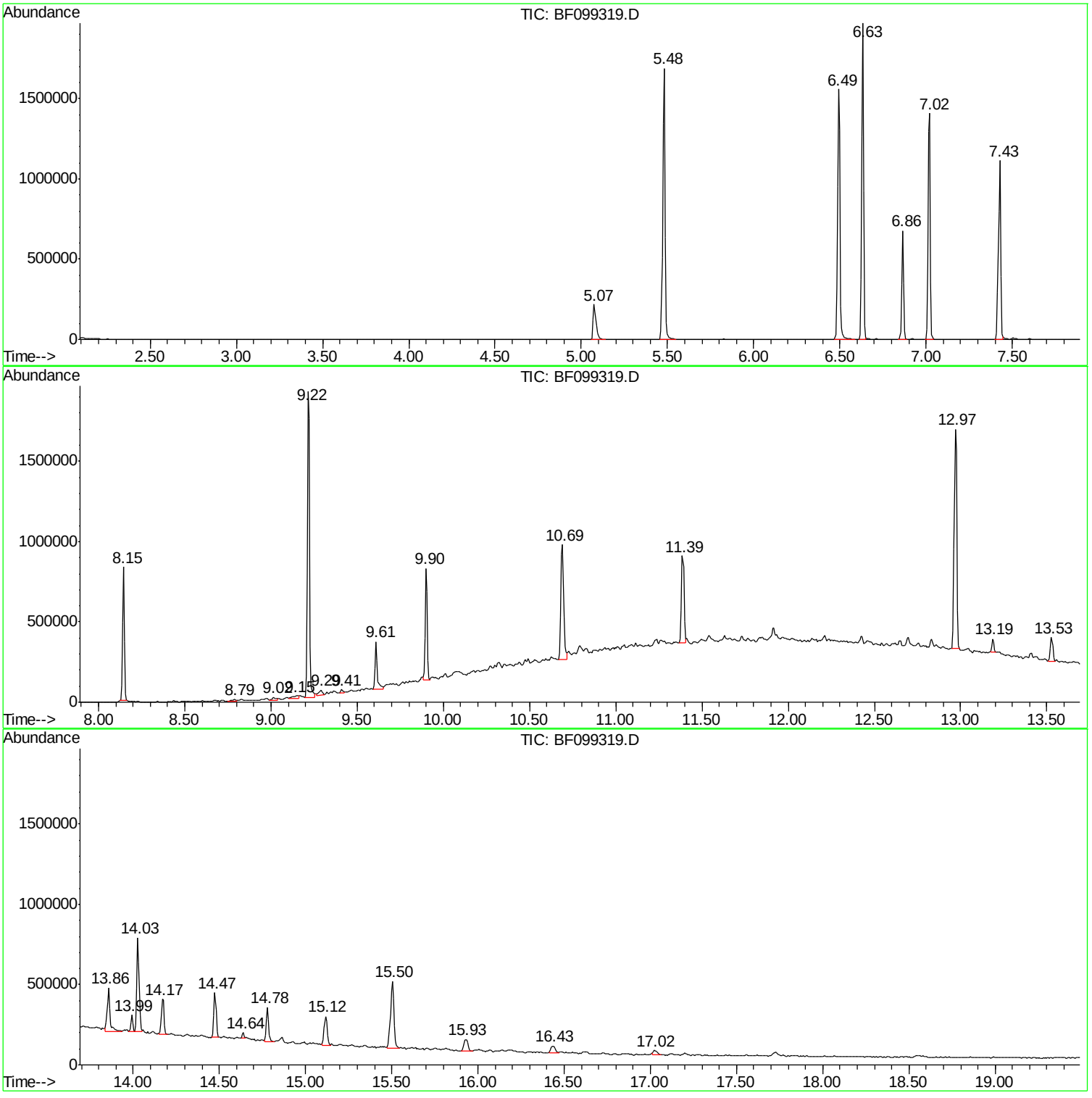
Sum of corrected areas: 16471142

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101017\
Data File : BF099319.D
Acq On : 11 Oct 2017 00:12
Operator : SJ/JU
Sample : I5691-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-115-8(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101017\
Data File : BF099319.D
Acq On : 11 Oct 2017 00:12
Operator : SJ/JU
Sample : I5691-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-115-8(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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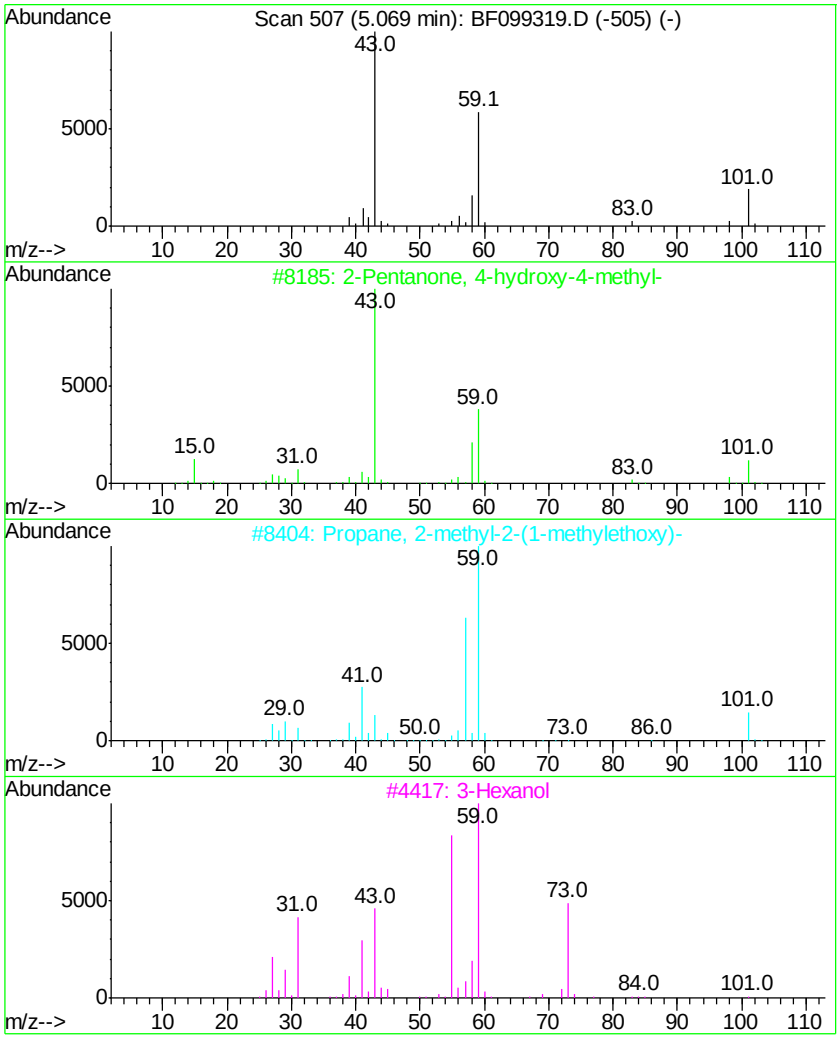
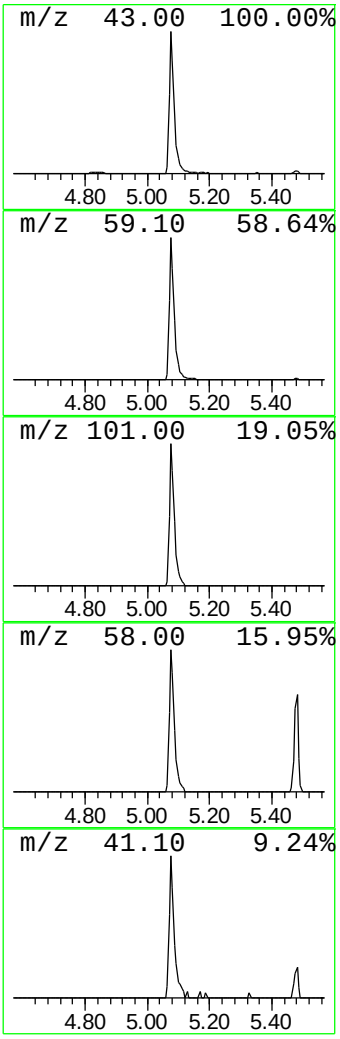
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	9.46 ng	248498	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Operator : SJ/JU
Sample : I5691-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-115-8(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

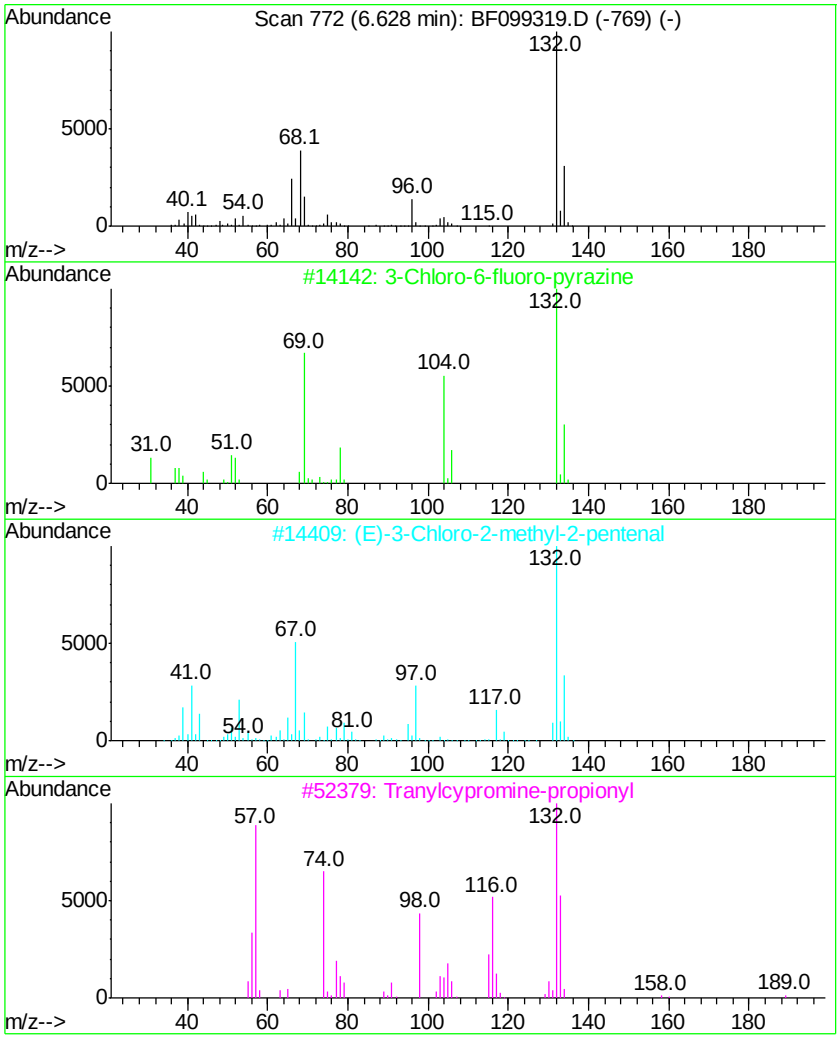
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

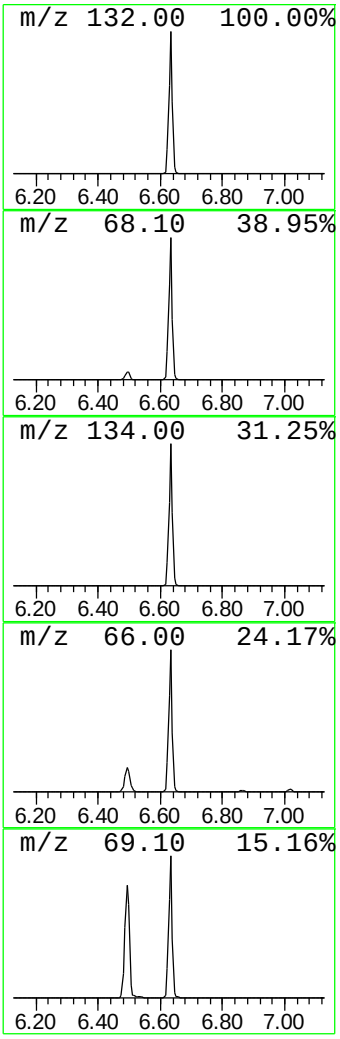
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	62.65 ng	1646080	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Operator : SJ/JU
Sample : I5691-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-115-8(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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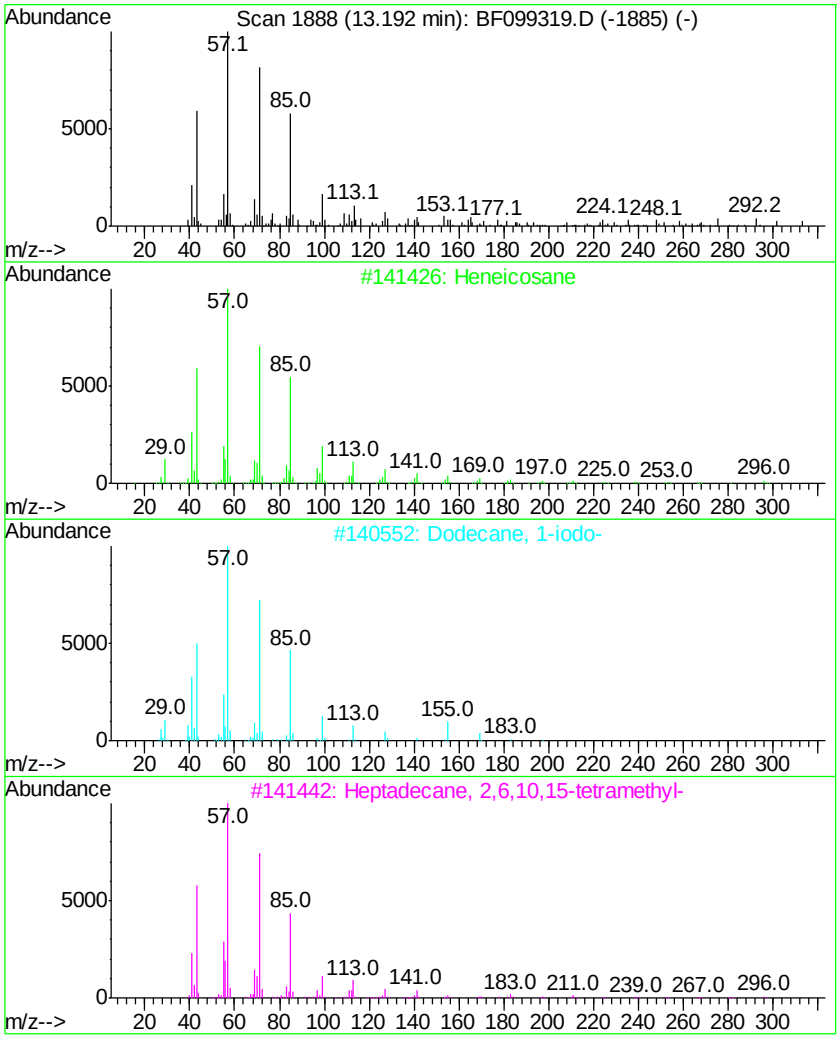
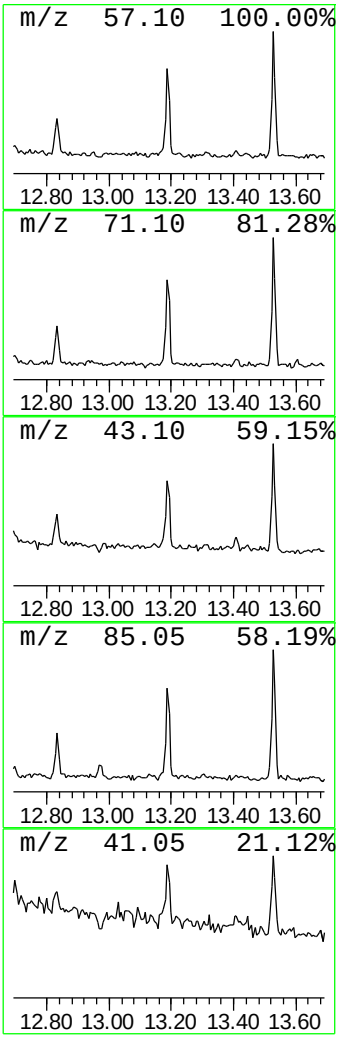
Peak Number 4 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	2.82 ng	72323	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	78
4	Hexadecane, 6,11-dipentyl-	366	C26H54	015874-03-0	72
5	Eicosane, 10-hexyl-10-methyl-	380	C27H56	055282-32-1	72





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Sample : I5691-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-115-8(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
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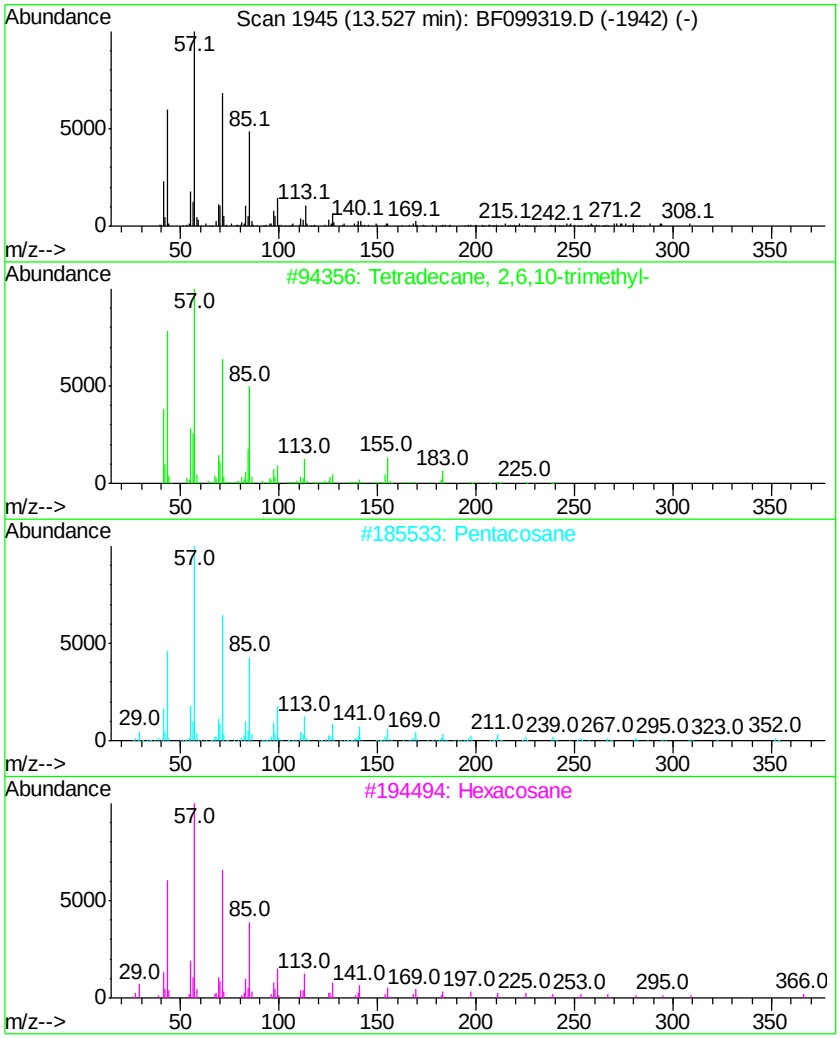
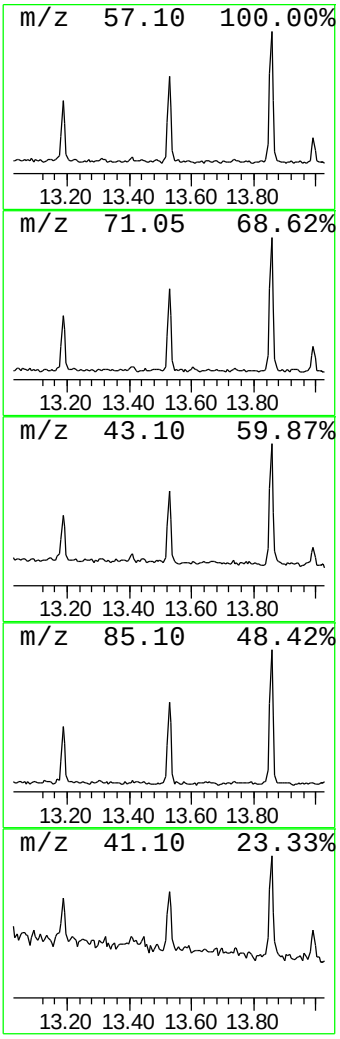
Peak Number 5 Tetradecane, 2,6,10-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	5.02 ng	128940	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	93
2	Pentacosane	352	C25H52	000629-99-2	90
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heptadecane	240	C17H36	000629-78-7	87
5	Heneicosane	296	C21H44	000629-94-7	87





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Sample : I5691-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-115-8(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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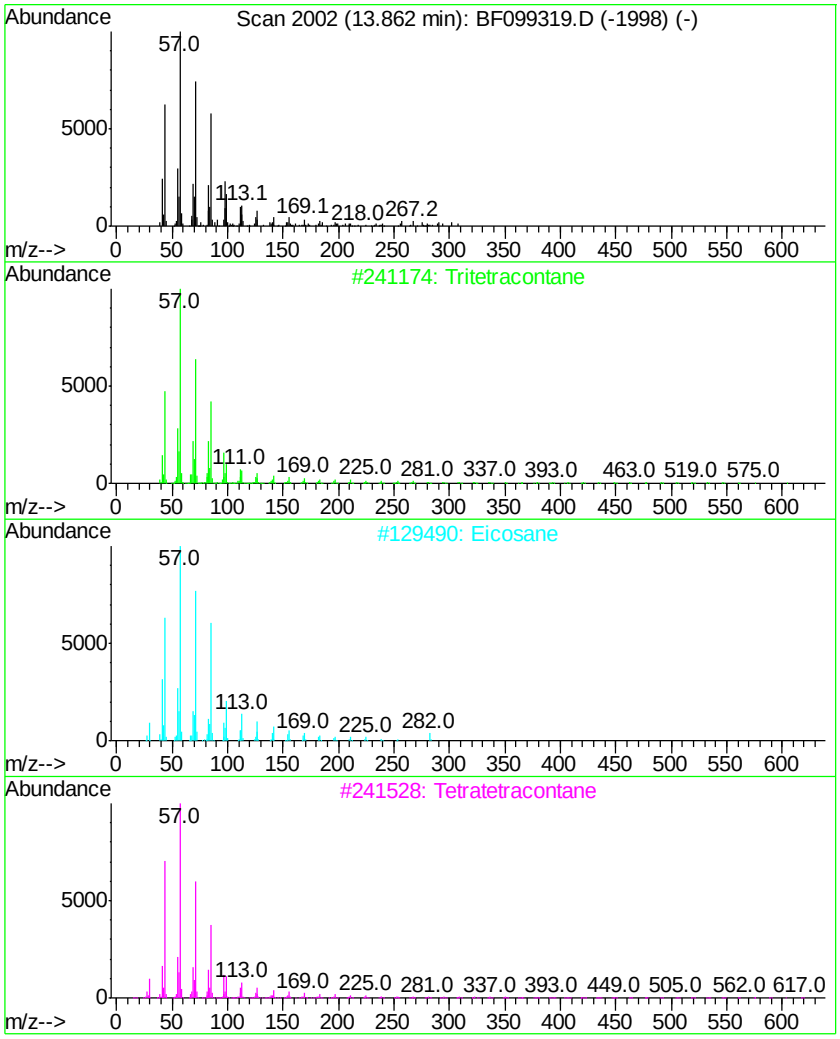
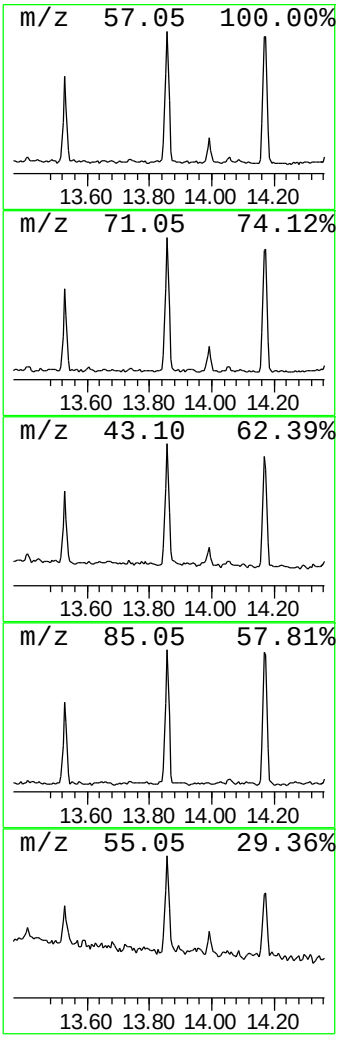
Peak Number 6 Tritetracontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	11.26 ng	289161	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tritetracontane	605	C43H88	007098-21-7	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	91





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Sample : I5691-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-115-8(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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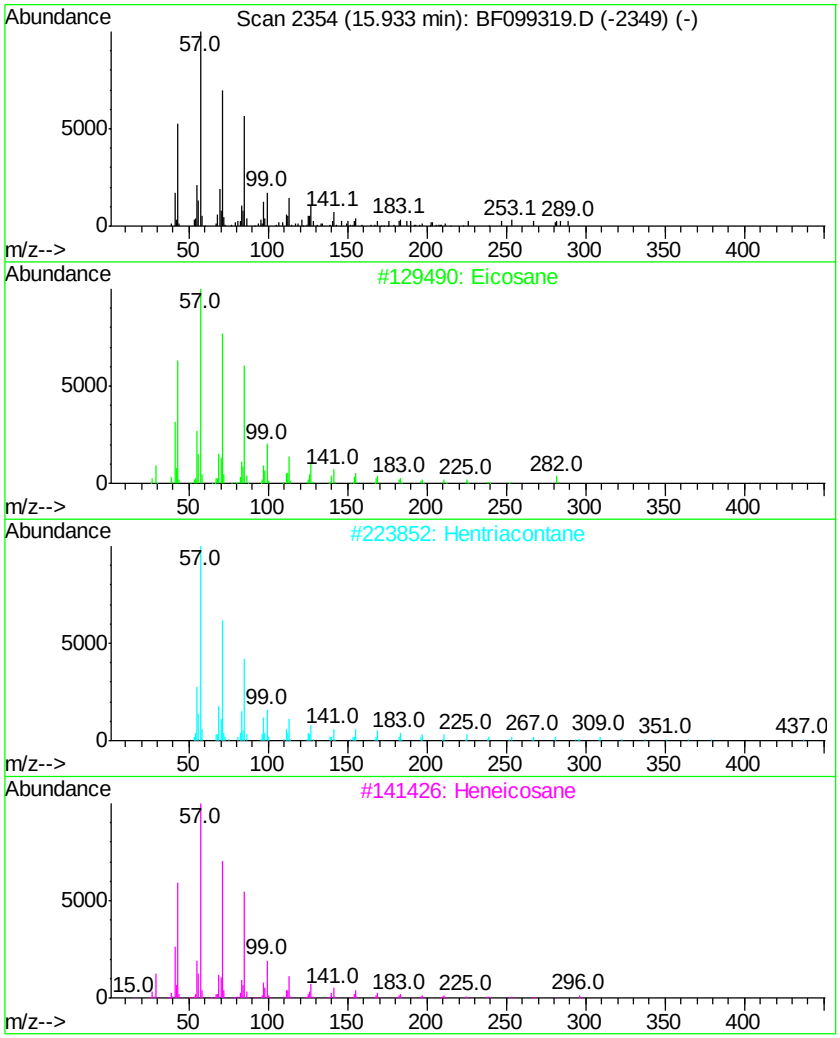
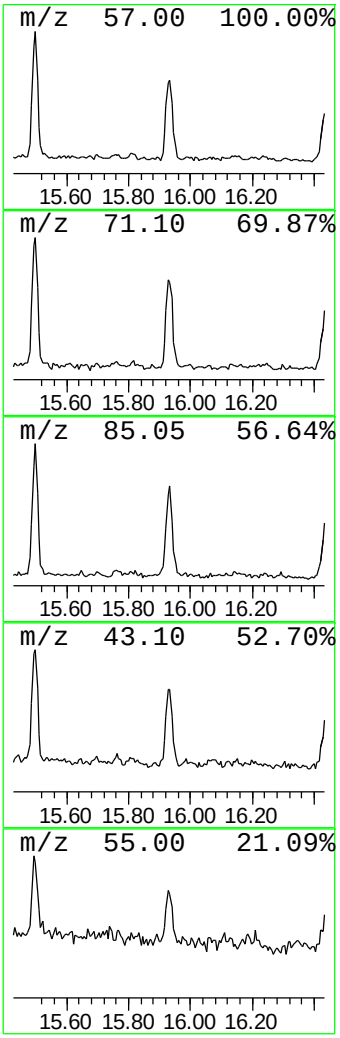
Peak Number 11 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	3.94 ng	111286	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Hexacosane	366	C26H54	000630-01-3	91





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...	5.07	9.5	ng	248498	1	6.86	525472	20.0
unknown6.63	6.63	62.6	ng	1646080	1	6.86	525472	20.0
Heneicosane	13.19	2.8	ng	72323	5	14.03	513713	20.0
Tetradecane, 2,6,...	13.53	5.0	ng	128940	5	14.03	513713	20.0
Tritetracontane	13.86	11.3	ng	289161	5	14.03	513713	20.0
Eicosane	15.93	3.9	ng	111286	6	15.50	564689	20.0