LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101017\
Data File : BF099298.D
Acq On : 10 Oct 2017 13:48
Operator : SJ/JU
Sample : I5651-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-1(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	2.163	9	13	19	rVB	25124	31635	1.76%	0.190%
2	5.087	507	510	524	rBV	238871	270947	15.04%	1.627%
3	5.487	574	578	593	rBV	1592298	1483444	82.35%	8.907%
4	6.492	744	749	752	rBV	1622677	1499144	83.23%	9.001%
5	6.633	769	773	776	rBV	1798919	1569541	87.13%	9.424%
6	6.863	808	812	815	rBV	673245	553189	30.71%	3.321%
7	7.016	834	838	842	rBV	1399117	1239067	68.79%	7.440%
8	7.428	903	908	911	rBV	943299	926777	51.45%	5.565%
9	7.498	916	920	928	rVB3	14233	22402	1.24%	0.135%
10	8.145	1025	1030	1033	rBV	863736	741392	41.16%	4.451%
11	9.216	1207	1212	1215	rBV	2131022	1801299	100.00%	10.815%
12	9.610	1275	1279	1286	rBV	287309	226640	12.58%	1.361%
13	9.898	1324	1328	1341	rVB2	927507	799577	44.39%	4.801%
14	10.316	1397	1399	1402	rVB	27901	21266	1.18%	0.128%
15	10.686	1458	1462	1470	rBV	1051072	926334	51.43%	5.562%
16	10.792	1476	1480	1489	rVB	37565	45695	2.54%	0.274%
17	11.386	1577	1581	1584	rBV	953345	800455	44.44%	4.806%
18	11.904	1665	1669	1673	rBV2	21257	23534	1.31%	0.141%
19	12.968	1845	1850	1853	rBV	1979962	1750570	97.18%	10.511%
20	13.186	1883	1887	1889	rBV	38854	34453	1.91%	0.207%
21	13.439	1926	1930	1934	rBV	26502	26898	1.49%	0.162%
22	13.492	1935	1939	1942	rVV	50819	45348	2.52%	0.272%
23	13.527	1942	1945	1948	rVB3	25566	24847	1.38%	0.149%
24	13.804	1988	1992	1997	rBV4	16760	29943	1.66%	0.180%
25	13.857	1997	2001	2011	rVB2	88364	146748	8.15%	0.881%
26	13.986	2020	2023	2026	rVB	102393	98660	5.48%	0.592%
27	14.027	2026	2030	2033	rBV	697501	678420	37.66%	4.073%
28	14.168	2051	2054	2057	rBV	38257	35534	1.97%	0.213%
29	14.474	2103	2106	2109	rBV	42891	37473	2.08%	0.225%
30	14.633	2130	2133	2137	rBV	87319	81416	4.52%	0.489%
31	14.780	2154	2158	2164	rVB2	38104	48226	2.68%	0.290%
32	14.862	2168	2172	2179	rVB5	12291	22782	1.26%	0.137%
33	15.115	2210	2215	2221	rVB	56242	66950	3.72%	0.402%
34	15.498	2275	2280	2290	rVB	366747	493272	27.38%	2.962%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.927	2349	2353	2361	rVB2	17885	28585	1.59%	0.172%
36	16.427	2433	2438	2447	rVB5	12476	22574	1.25%	0.136%

Sum of corrected areas: 16655037

LSC Report - Integrated Chromatogram

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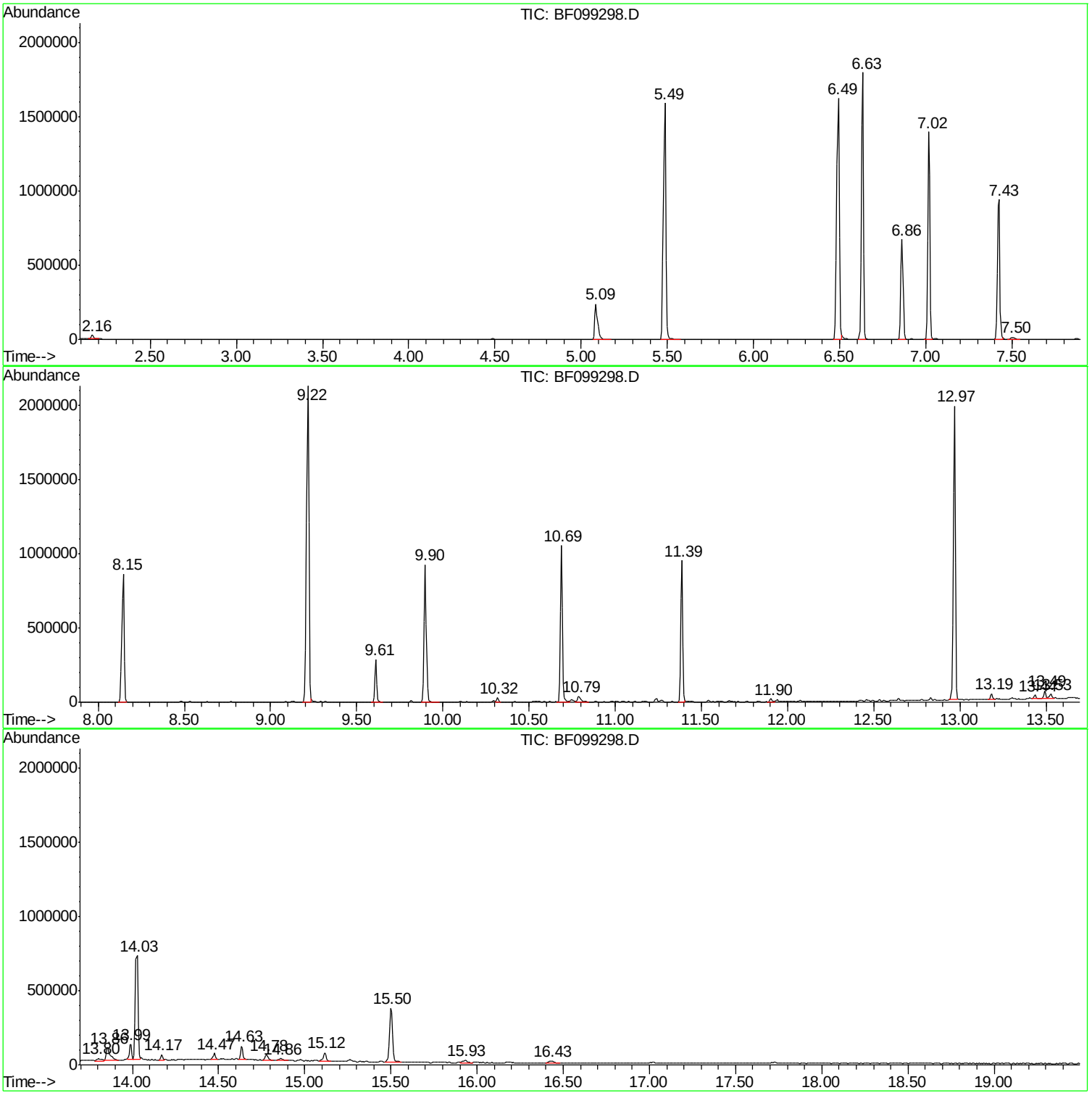
Sample : I5651-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-116-1(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 : BF099298.D
Acq On : 10 Oct 2017 13:48
Operator : SJ/JU
Sample : I5651-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-1(5-10)

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

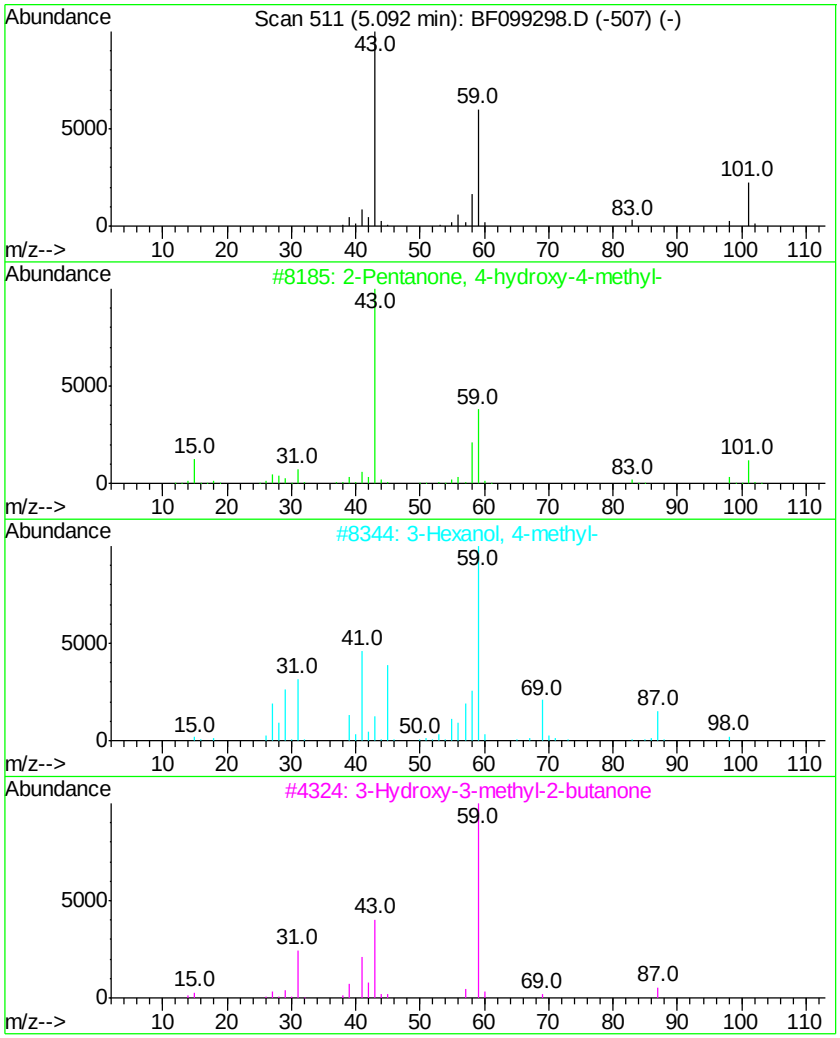
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

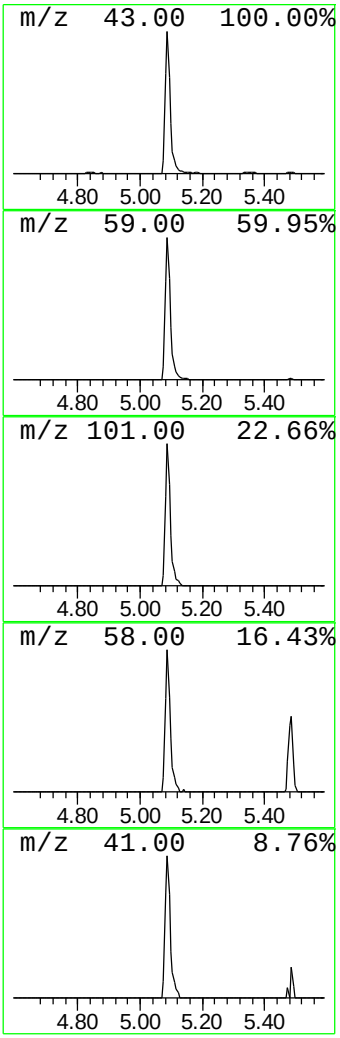
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	9.80 ng	270947	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	53
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9





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Acq On : 10 Oct 2017 13:48
Operator : SJ/JU
Sample : I5651-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-1(5-10)

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

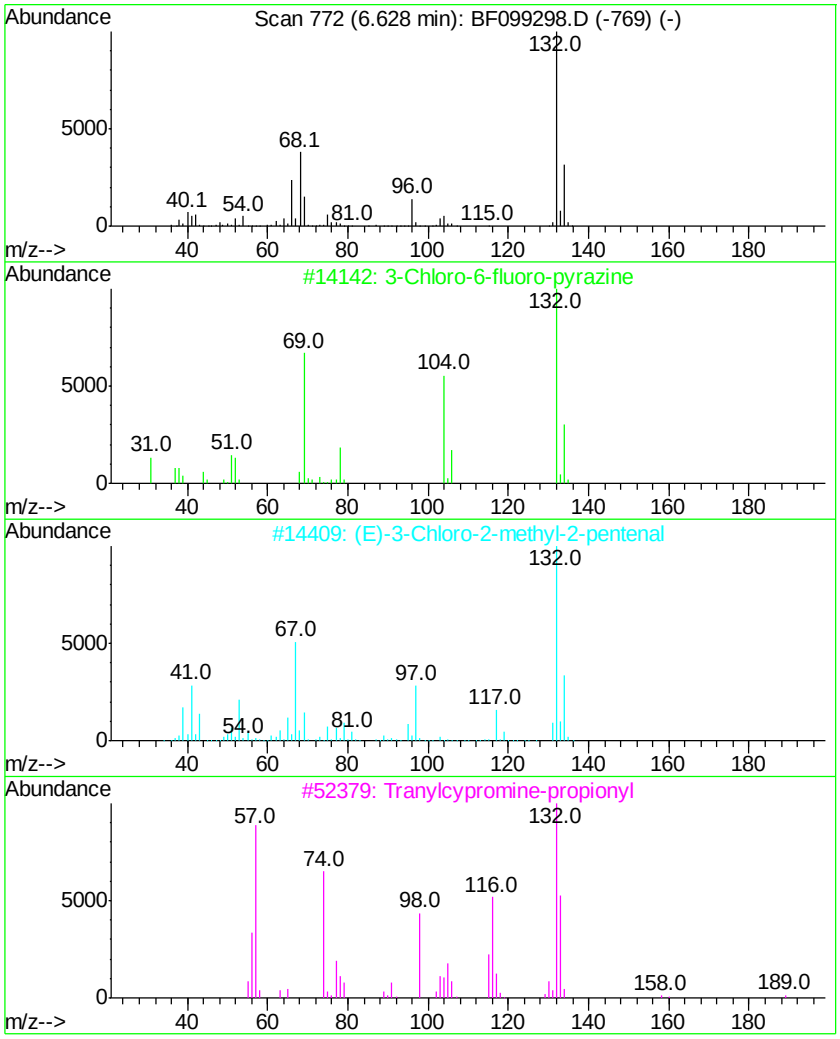
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

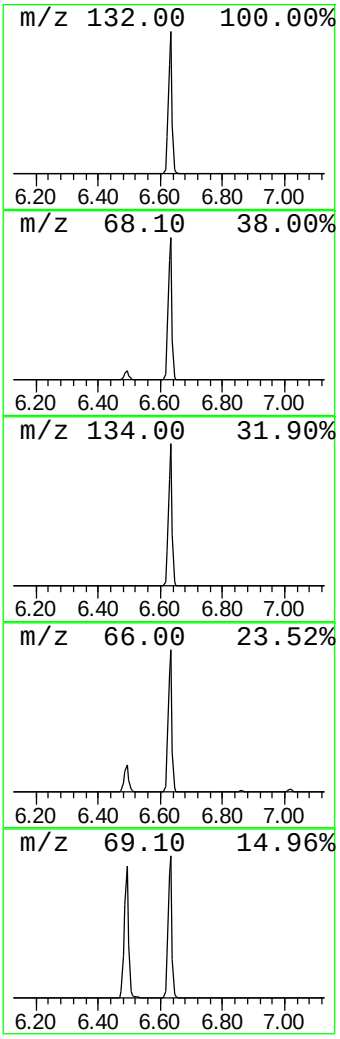
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	56.75 ng	1569540	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	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101017\
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-1(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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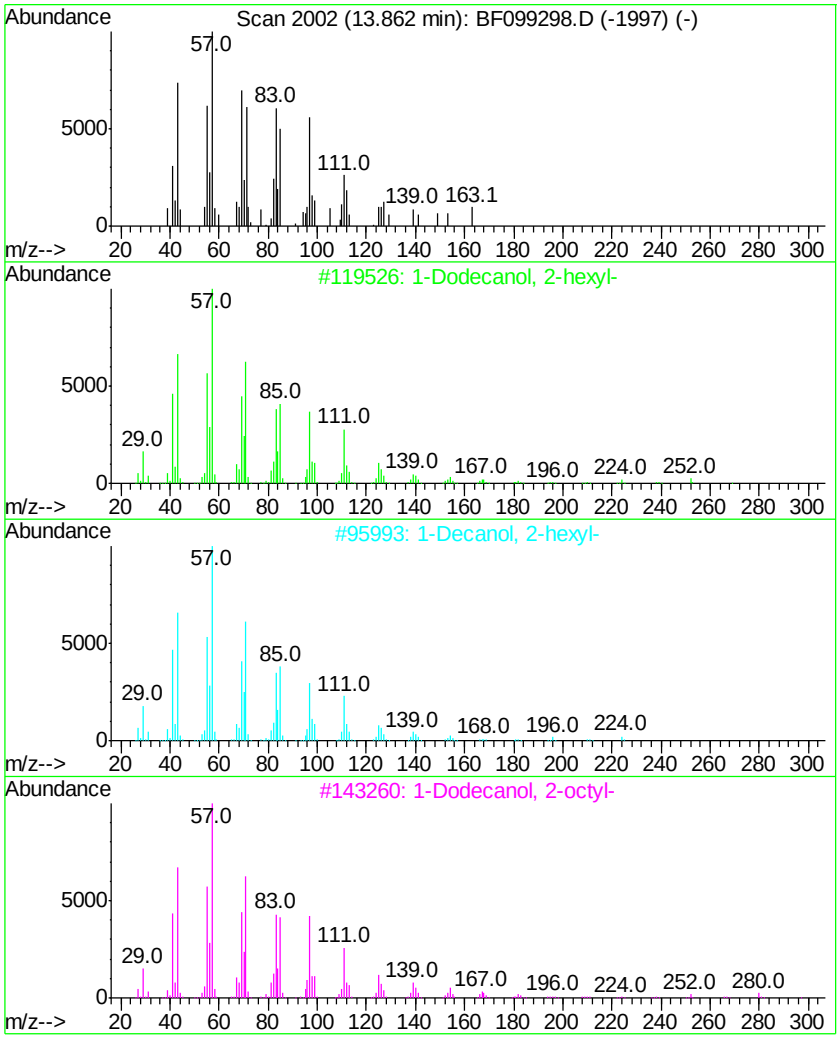
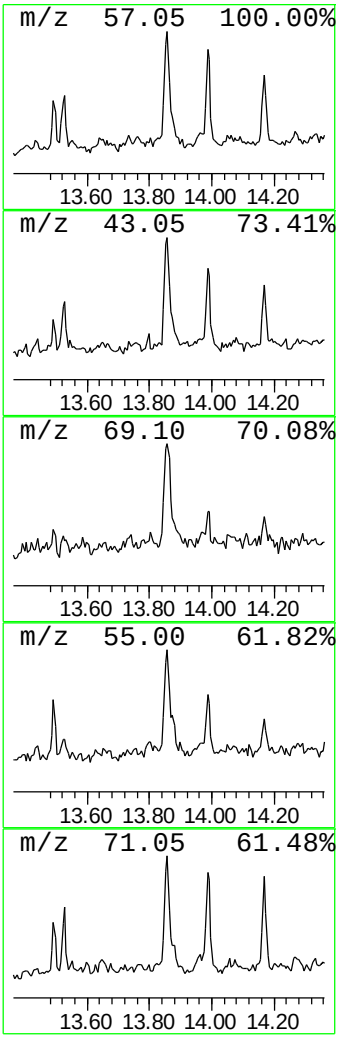
Peak Number 4 1-Dodecanol, 2-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	4.33 ng	146748	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	90
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	90
3	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	87
4	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	81
5	Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	64





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-1(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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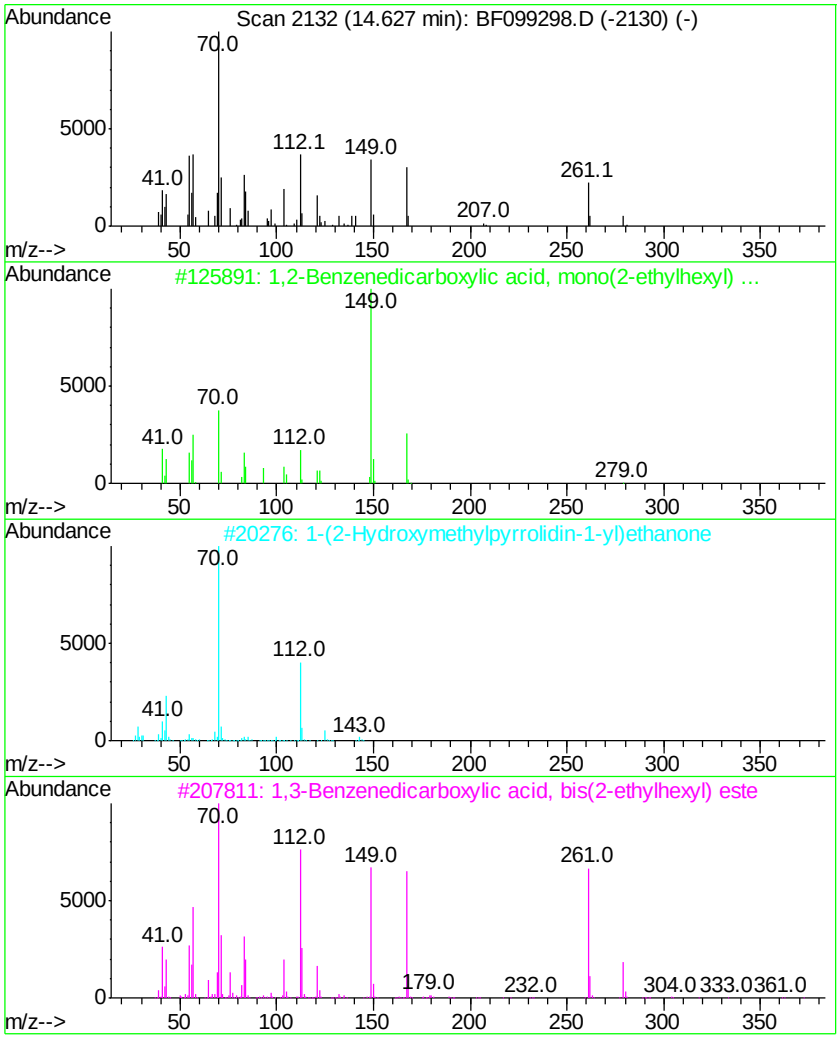
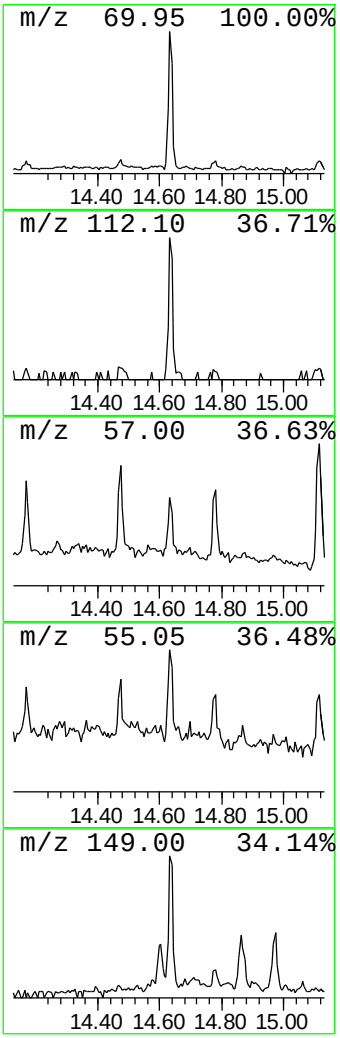
****

Peak Number 5 unknown14.63 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	2.40 ng	81416	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	43
2	1-(2-Hydroxymethylpyrrolidin-1-y...	143	C7H13NO2	1000192-83-2	25
3	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	25
4	Dimethylmalonic acid, monochlori...	262	C13H23ClO3	1000361-64-8	25
5	5-Chloropentanoic acid, 2-ethylh...	248	C13H25ClO2	1000293-48-9	22





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

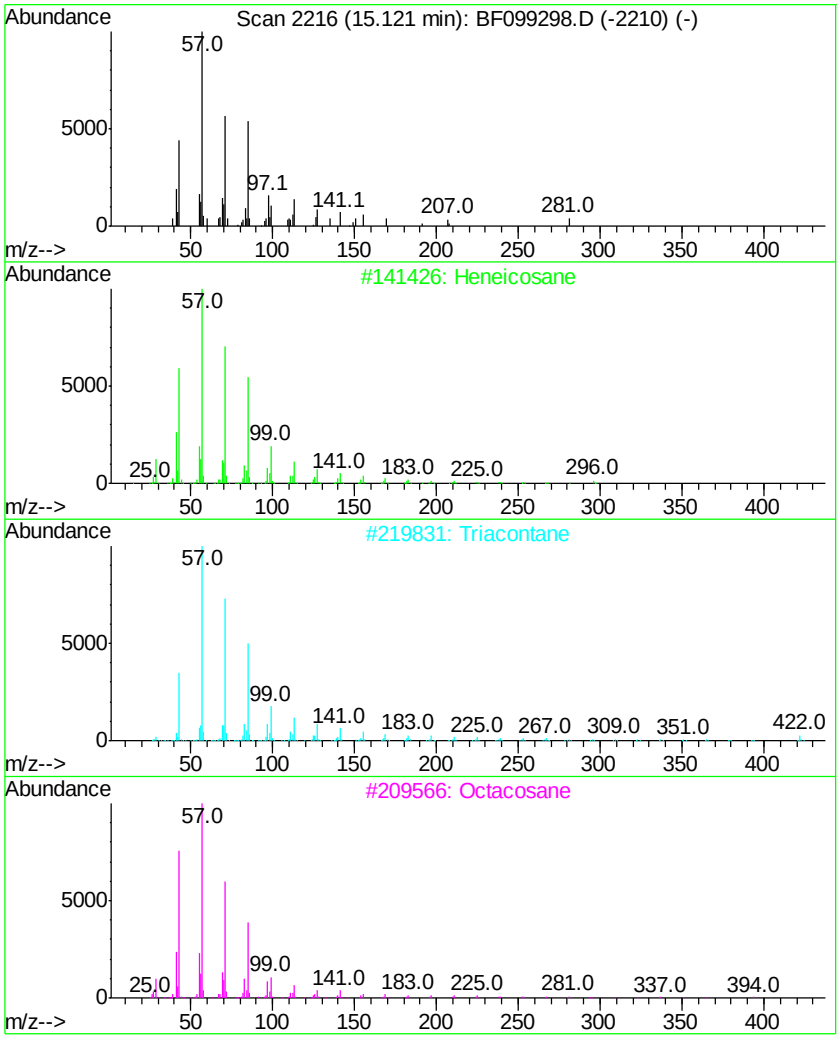
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

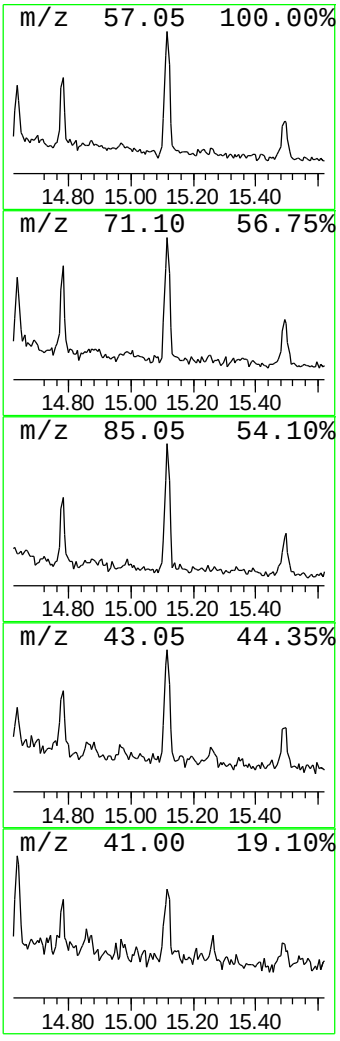
****

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	2.71 ng	66950	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Triacontane	422	C30H62	000638-68-6	91
3	Octacosane	394	C28H58	000630-02-4	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Tentatively Identified Compound (LSC) summary

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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...	5.09	9.8	ng	270947	1	6.86	553189	20.0
unknown6.63	6.63	56.8	ng	1569540	1	6.86	553189	20.0
1-Dodecanol, 2-he...	13.86	4.3	ng	146748	5	14.03	678420	20.0
unknown14.63	14.63	2.4	ng	81416	5	14.03	678420	20.0
Heneicosane	15.12	2.7	ng	66950	6	15.50	493272	20.0