LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100317\
Data File : BF099058.D
Acq On : 4 Oct 2017 4:11
Operator : SJ/JU
Sample : I5588-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-EPE-T8(0-5)

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	2.157	8	12	18	rVB	139661	186125	5.85%	0.703%
2	5.098	509	512	526	rVB	471889	667624	20.98%	2.521%
3	5.498	574	580	583	rBV	2972415	3181933	100.00%	12.016%
4	6.504	745	751	754	rBV	2789363	3082987	96.89%	11.643%
5	6.645	770	775	778	rBV	3225678	3151772	99.05%	11.902%
6	6.875	808	814	817	rBV	959088	804915	25.30%	3.040%
7	6.998	833	835	837	rBV	55022	50626	1.59%	0.191%
8	7.033	837	841	844	rVB	2592383	2422462	76.13%	9.148%
9	7.439	904	910	913	rBV	1986058	1855115	58.30%	7.006%
10	8.157	1028	1032	1035	rBV	973171	836835	26.30%	3.160%
11	9.227	1209	1214	1217	rBV	3099471	2796819	87.90%	10.562%
12	9.616	1277	1280	1284	rBV	394126	334494	10.51%	1.263%
13	9.910	1326	1330	1334	rVB	822098	670953	21.09%	2.534%
14	10.698	1460	1464	1467	rBV	1335106	1150584	36.16%	4.345%
15	10.804	1479	1482	1489	rBV	33660	34105	1.07%	0.129%
16	11.392	1579	1582	1586	rBV	637827	562257	17.67%	2.123%
17	11.610	1614	1619	1626	rBV2	50118	51669	1.62%	0.195%
18	12.427	1754	1758	1764	rBV	352095	316249	9.94%	1.194%
19	12.486	1765	1768	1773	rVB2	32215	32178	1.01%	0.122%
20	12.980	1847	1852	1855	rBV	2546625	2207442	69.37%	8.336%
21	13.174	1882	1885	1894	rBV	78796	99797	3.14%	0.377%
22	13.415	1923	1926	1930	rBV	146066	117607	3.70%	0.444%
23	13.862	1999	2002	2010	rBV	229942	246657	7.75%	0.931%
24	14.004	2020	2026	2028	rBV	142191	116469	3.66%	0.440%
25	14.033	2028	2031	2035	rVB	799143	703557	22.11%	2.657%
26	14.492	2105	2109	2117	rBV7	23028	44566	1.40%	0.168%
27	15.509	2277	2282	2292	rVB	605308	721622	22.68%	2.725%
28	16.015	2363	2368	2375	rBV9	15063	32589	1.02%	0.123%

Sum of corrected areas: 26480008

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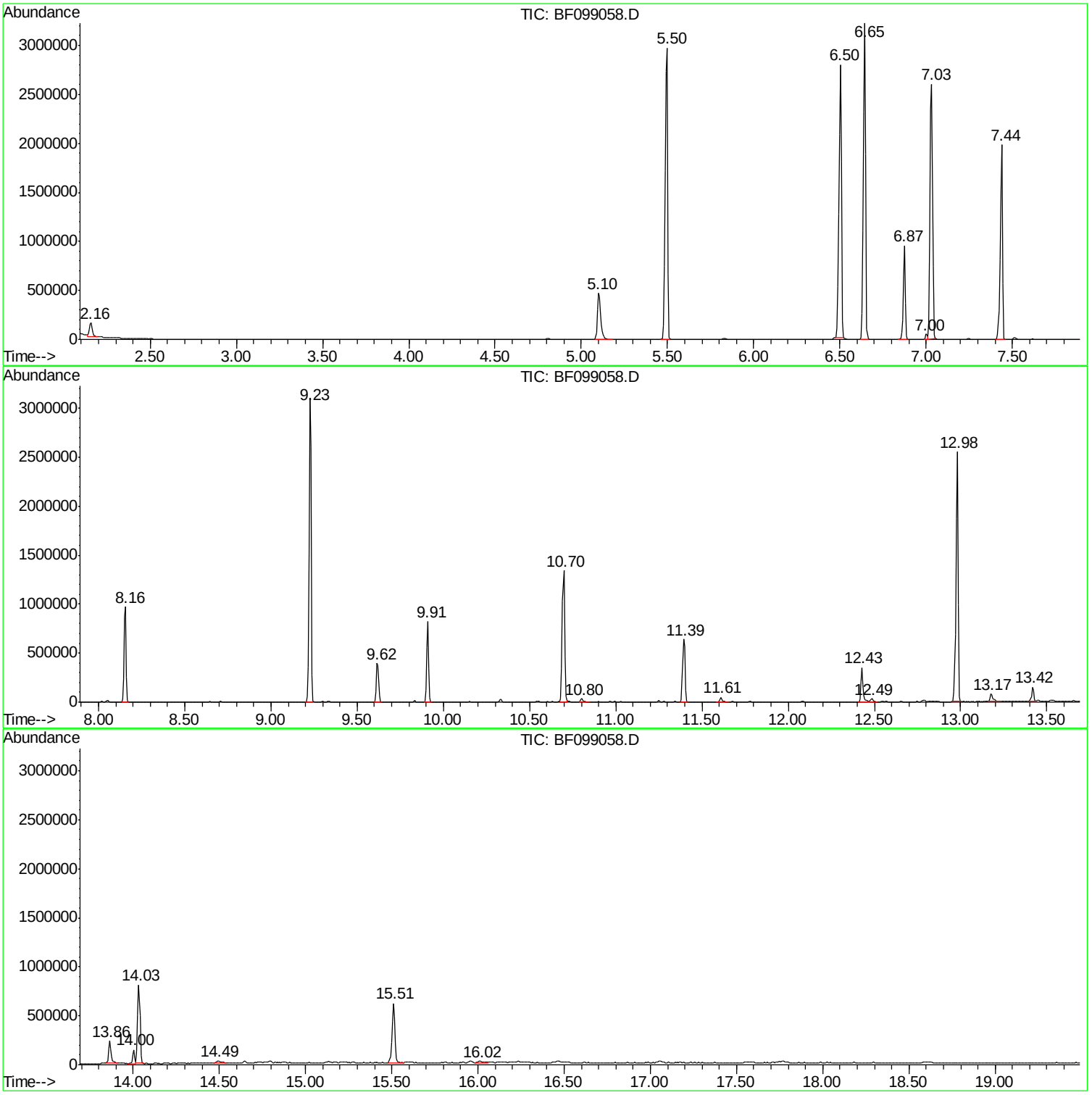
Instrument :
BNA_F
ClientSampleId :
SASP2P-EPE-T8(0-5)

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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TIC Library : C:\DATABASE\NIST11.L
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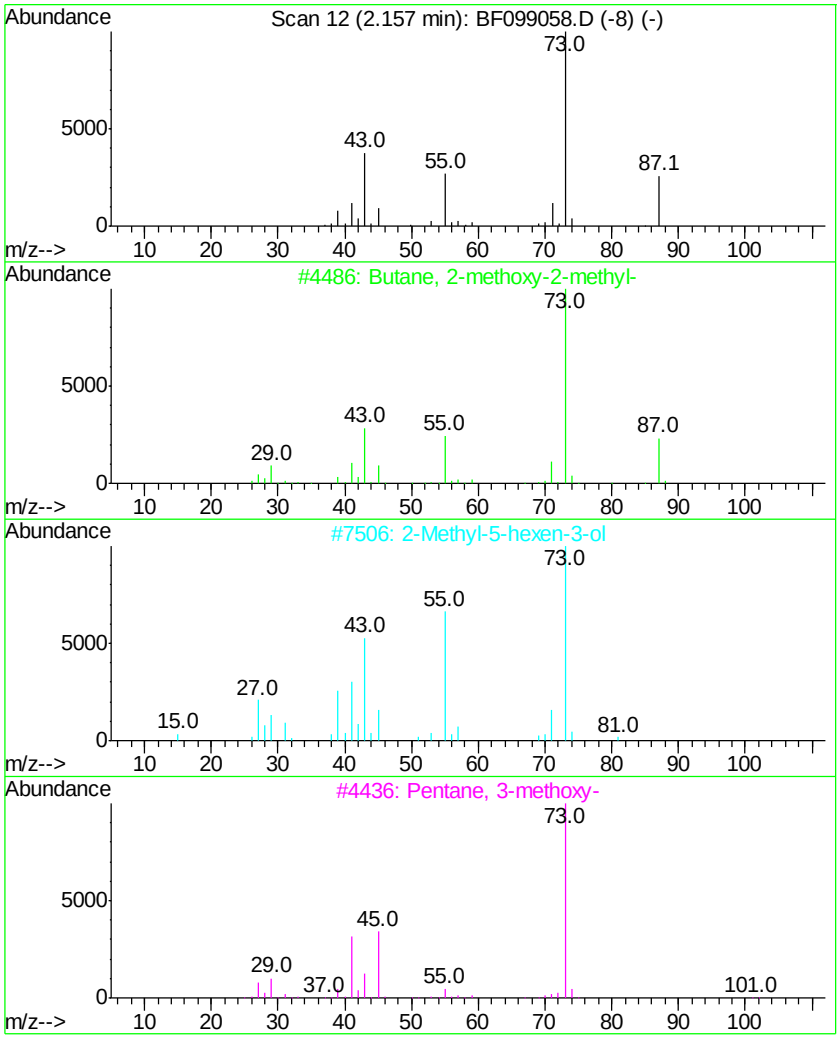
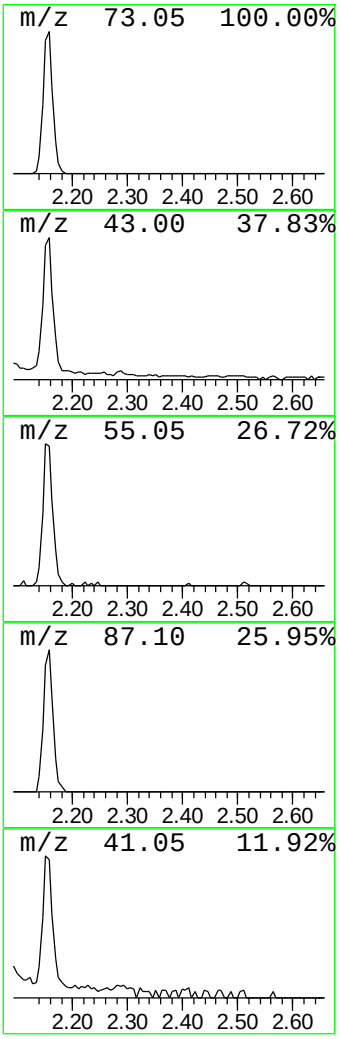
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	4.62 ng	186125	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	25
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	16
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Sample : I5588-03
Misc :
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Instrument : BNA_F
ClientSampleId : SASP2P-EPE-T8(0-5)

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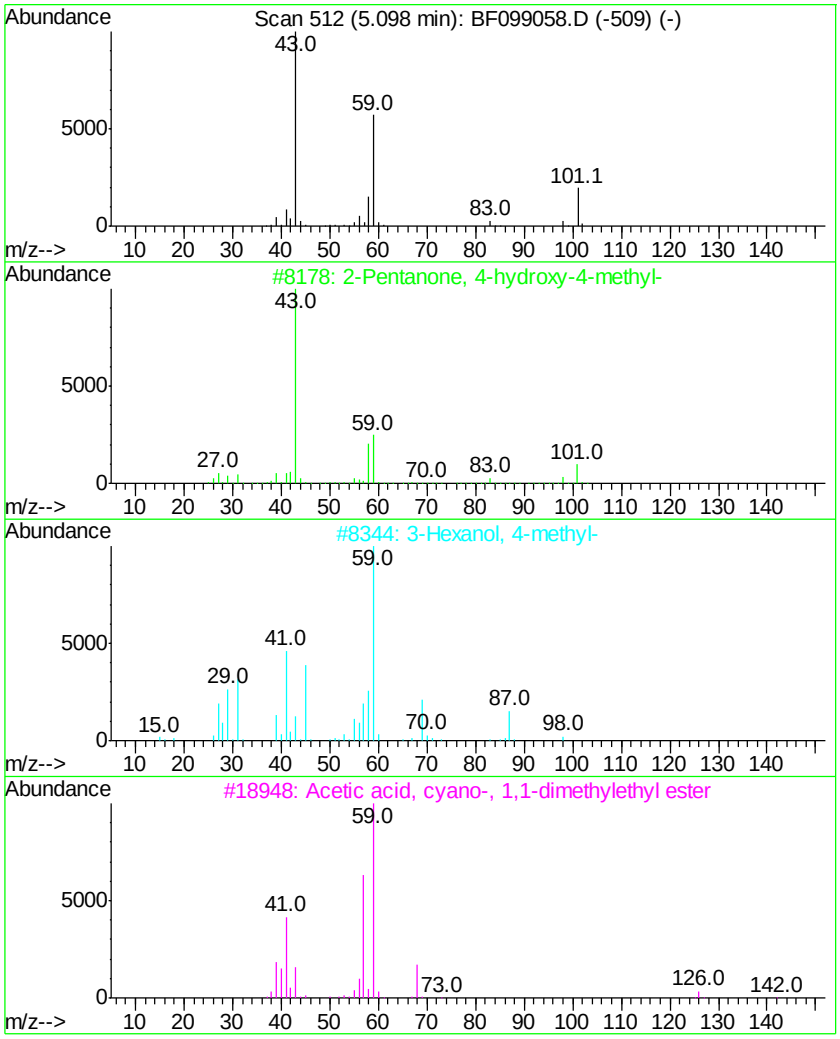
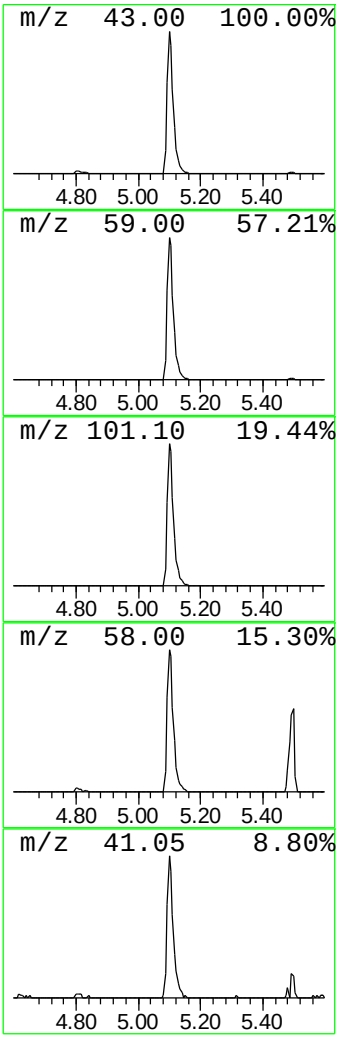
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	16.59 ng	667624	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument : BNA_F
ClientSampleId : SASP2P-EPE-T8(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Integration Parameters: LSCINT.P

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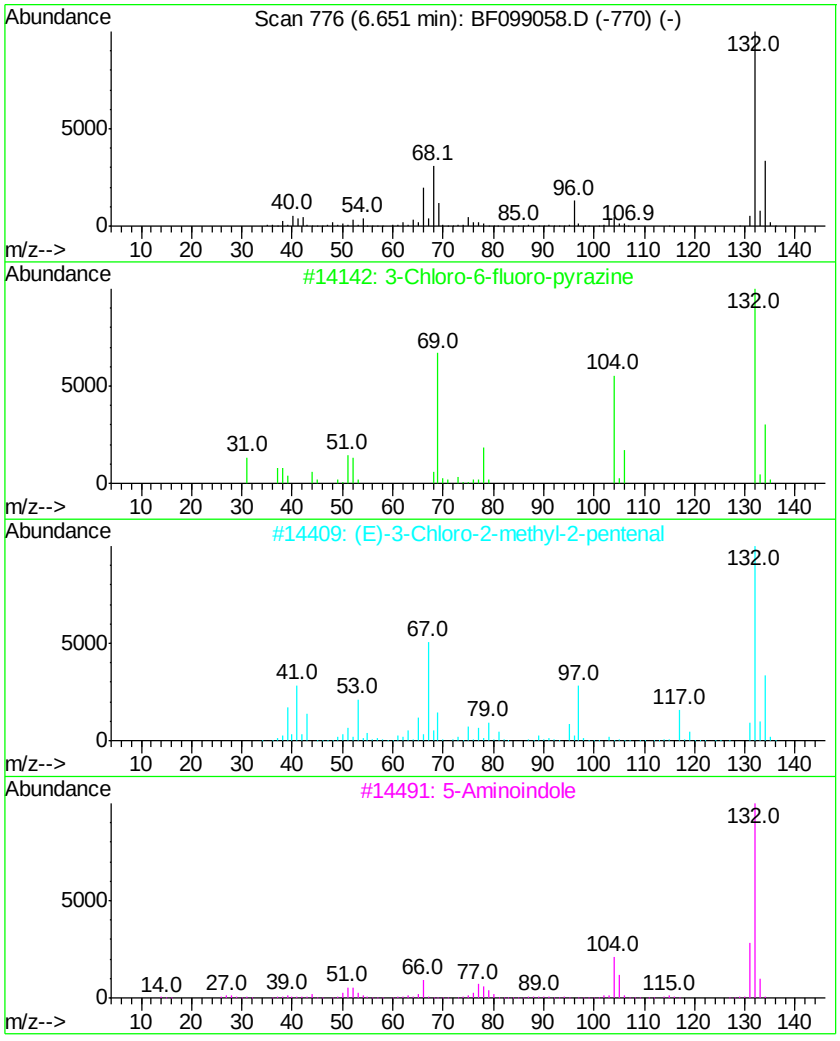
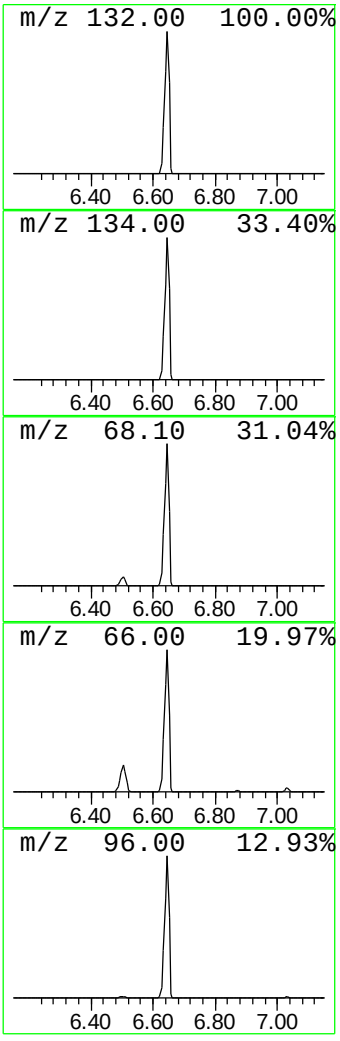
Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	78.31 ng	3151770	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Sample : I5588-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-EPE-T8(0-5)

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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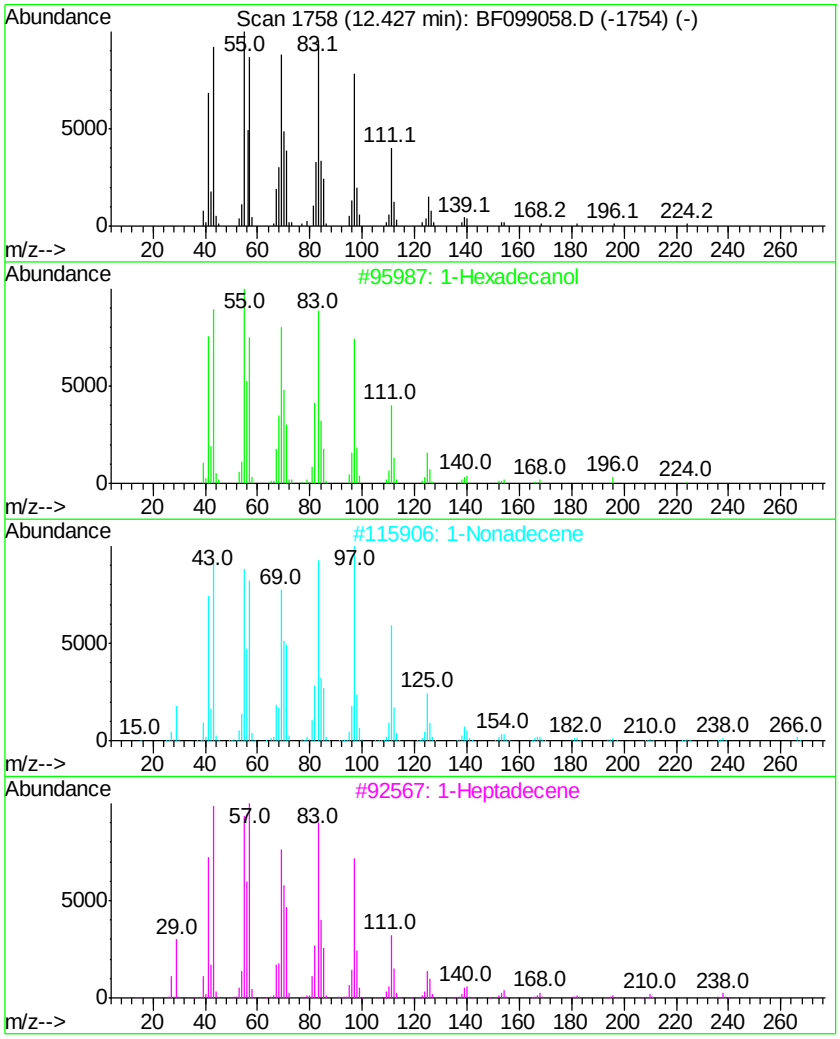
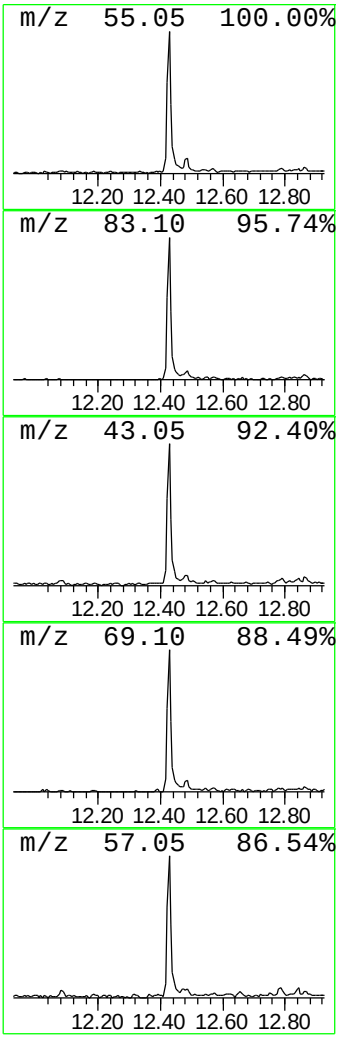
Peak Number 5 1-Hexadecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	11.25 ng	316249	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	93
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	1-Heptadecene	238	C17H34	006765-39-5	91
4	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	91
5	9-Octadecene, (E)-	252	C18H36	007206-25-9	91





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Operator : SJ/JU
Sample : I5588-03
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-EPE-T8(0-5)

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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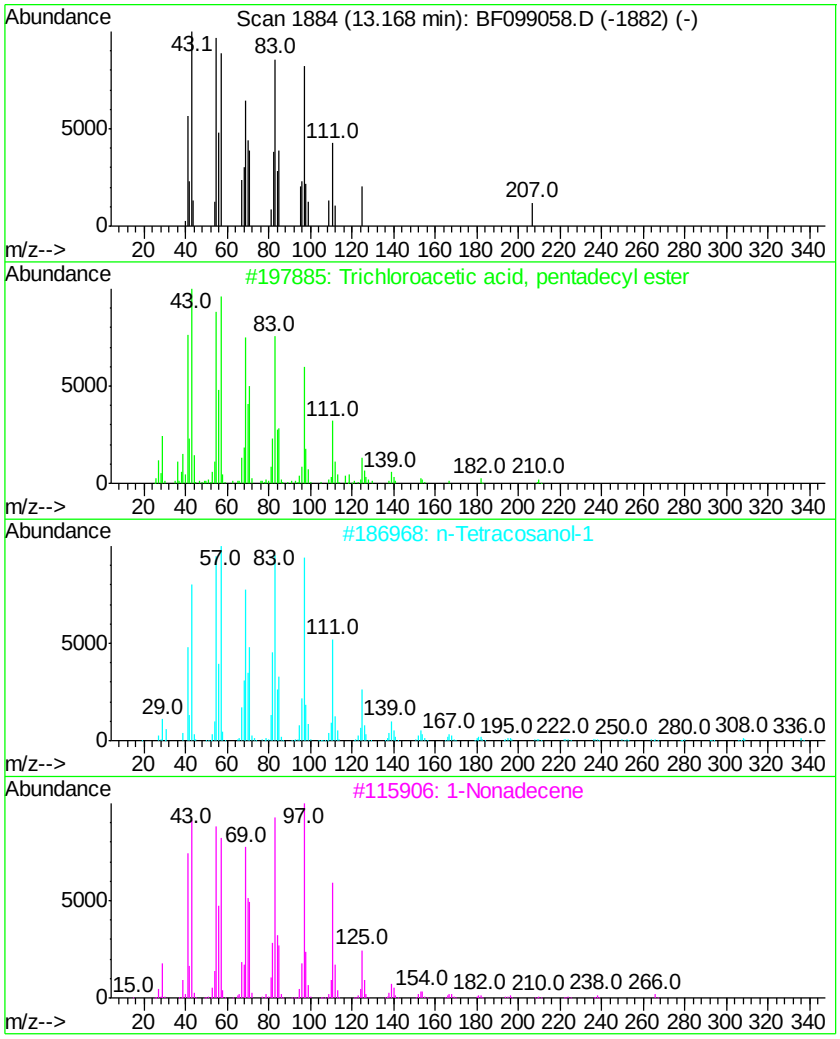
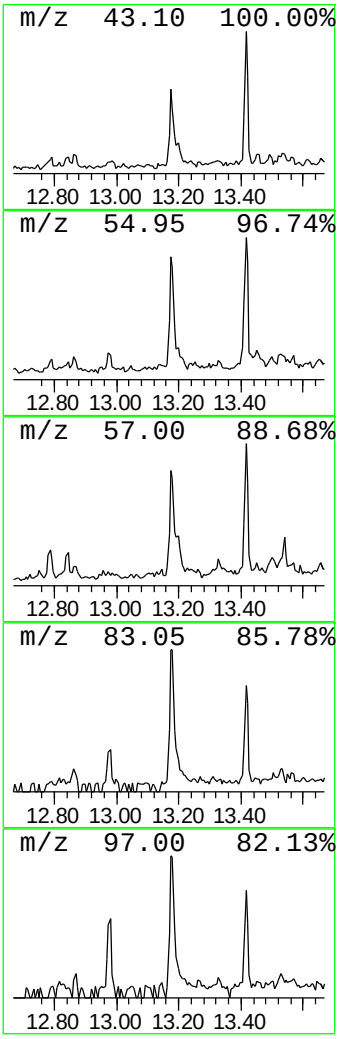
Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.17	2.84 ng	99797	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





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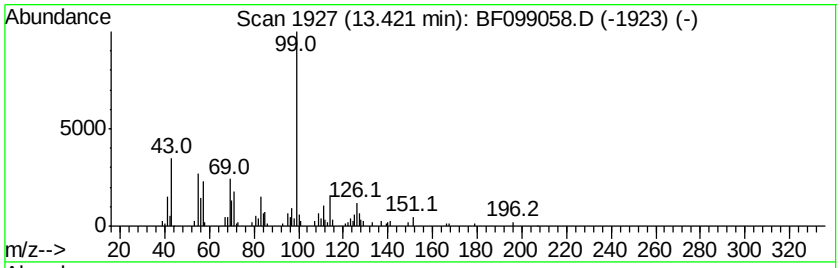
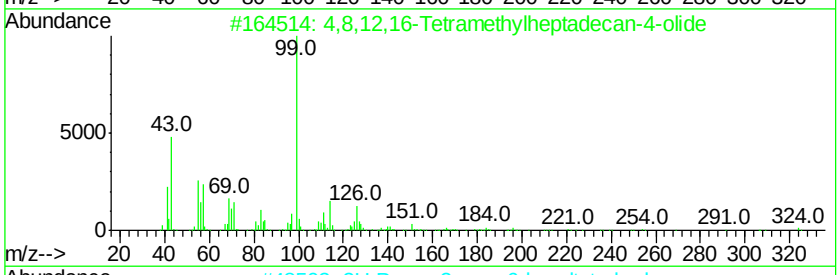
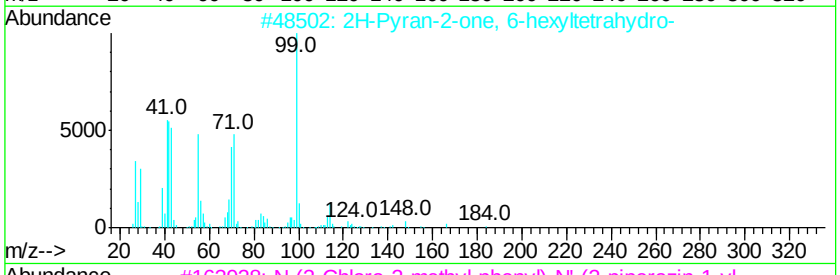
Peak Number 7 4,8,12,16-Tetramethylheptad... Concentration Rank 7

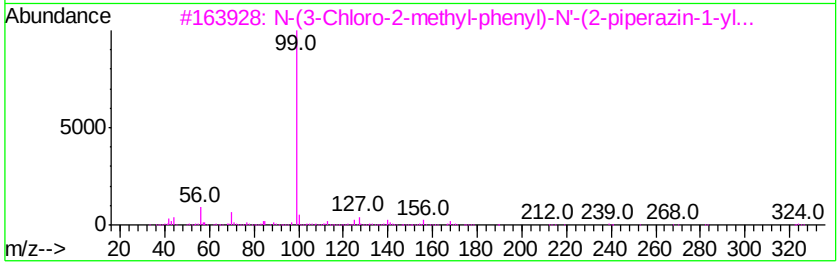
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.42	3.34 ng	117607	Chrysene-d12	14.03

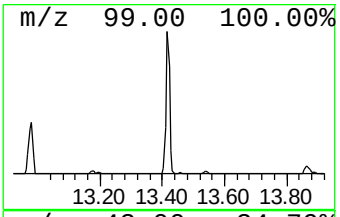
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	91
2	2H-Pyran-2-one, 6-hexyltetrahydro-	184	C11H20O2	000710-04-3	53
3	N-(3-Chloro-2-methyl-phenyl)-N'-...	324	C15H21ClN4O2	1000294-79-6	50
4	Hexanoic acid, 4-hexadecyl ester	340	C22H44O2	1000282-83-8	50
5	2H-Pyran-2-one, 6-heptyltetrahydro-	198	C12H22O2	000713-95-1	50

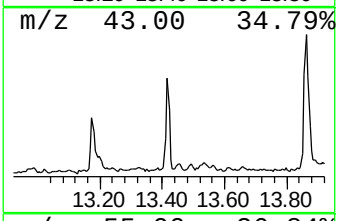


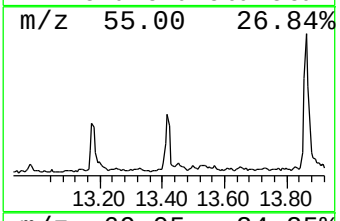


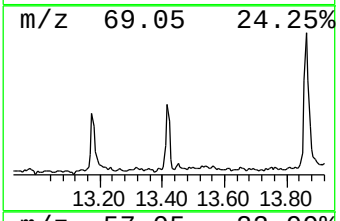


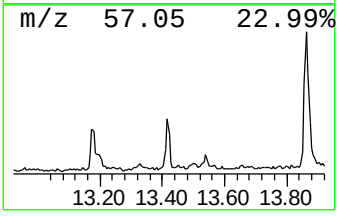












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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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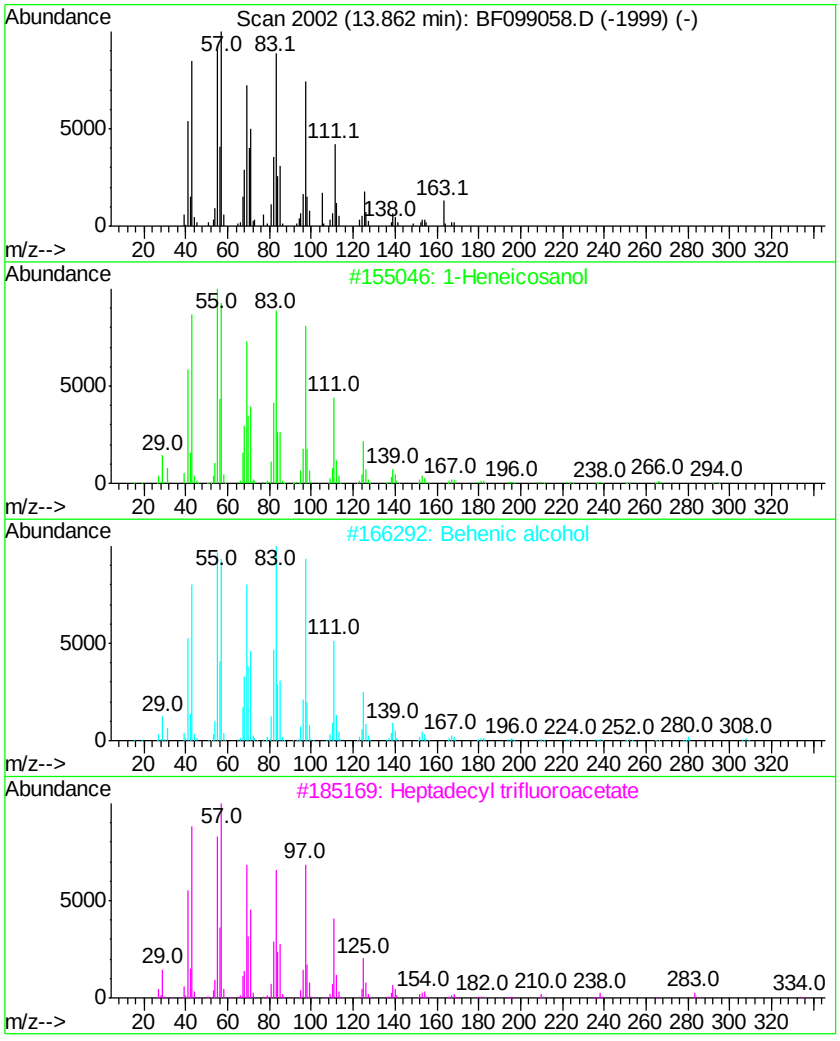
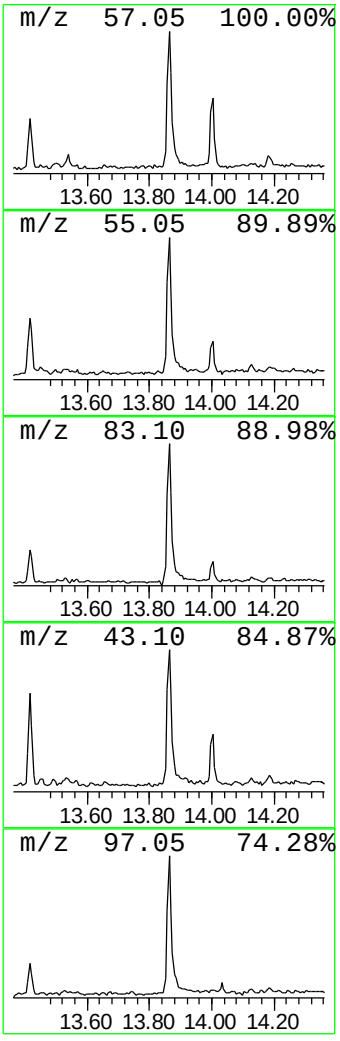
Peak Number 8 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	7.01 ng	246657	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93





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
Butane, 2-methoxy...	2.16	4.6	ng	186125	1	6.87	804915	20.0
2-Pentanone, 4-hy...	5.10	16.6	ng	667624	1	6.87	804915	20.0
unknown6.65	6.65	78.3	ng	3151770	1	6.87	804915	20.0
1-Hexadecanol	12.43	11.3	ng	316249	4	11.39	562257	20.0
Trichloroacetic a...	13.17	2.8	ng	99797	5	14.03	703557	20.0
4,8,12,16-Tetrame...	13.42	3.3	ng	117607	5	14.03	703557	20.0
1-Heneicosanol	13.86	7.0	ng	246657	5	14.03	703557	20.0