LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098879.D
Acq On : 27 Sep 2017 22:56
Operator : SJ/JU
Sample : I5386-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-ENV-116-2(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	2.210	18	21	35	rVB2	110019	198495	5.94%	0.630%
2	5.145	515	520	533	rVB	522477	677285	20.27%	2.151%
3	5.539	581	587	590	rBV	3068692	3176144	95.07%	10.086%
4	6.539	752	757	760	rBV	2931759	3244425	97.11%	10.303%
5	6.686	777	782	785	rBV	3329896	3214751	96.22%	10.209%
6	6.916	815	821	824	rBV	1030980	910475	27.25%	2.891%
7	7.069	843	847	851	rVB	2673048	2481585	74.28%	7.880%
8	7.475	911	916	919	rBV	2047951	1994710	59.70%	6.334%
9	7.545	925	928	933	rVB	45810	45463	1.36%	0.144%
10	8.198	1035	1039	1042	rBV	1213981	1082594	32.40%	3.438%
11	9.269	1216	1221	1225	rBV	3480210	3340976	100.00%	10.610%
12	9.657	1284	1287	1291	rBV	537947	458401	13.72%	1.456%
13	9.951	1333	1337	1341	rBV2	1244692	1058158	31.67%	3.360%
14	10.374	1406	1409	1412	rVB	46416	36888	1.10%	0.117%
15	10.739	1467	1471	1474	rBV	1741290	1517945	45.43%	4.820%
16	10.845	1486	1489	1495	rBV	59159	58104	1.74%	0.185%
17	11.439	1586	1590	1593	rBV	1081920	885497	26.50%	2.812%
18	11.951	1674	1677	1686	rBV	156549	160413	4.80%	0.509%
19	12.651	1792	1796	1800	rBV	64239	62664	1.88%	0.199%
20	12.739	1807	1811	1819	rBV2	63099	79991	2.39%	0.254%
21	12.833	1824	1827	1830	rVB	56041	41739	1.25%	0.133%
22	12.880	1830	1835	1838	rBV	63728	63156	1.89%	0.201%
23	13.021	1855	1859	1862	rBV	2515880	2303109	68.94%	7.314%
24	13.862	1998	2002	2005	rBV2	23221	35815	1.07%	0.114%
25	13.904	2006	2009	2014	rVV2	143411	146248	4.38%	0.464%
26	14.045	2030	2033	2035	rBV	51834	50062	1.50%	0.159%
27	14.080	2035	2039	2042	rVV	839037	820623	24.56%	2.606%
28	14.533	2114	2116	2122	rVB4	34801	39619	1.19%	0.126%
29	14.698	2140	2144	2148	rBV	2559895	2387139	71.45%	7.581%
30	15.192	2226	2228	2239	rVB4	48942	83213	2.49%	0.264%
31	15.568	2287	2292	2302	rVB	558688	776678	23.25%	2.466%
32	16.027	2367	2370	2376	rVB	43851	57982	1.74%	0.184%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098879.D
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Operator : SJ/JU
Sample : I5386-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-116-2(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: 31490347

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098879.D
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Sample : I5386-02
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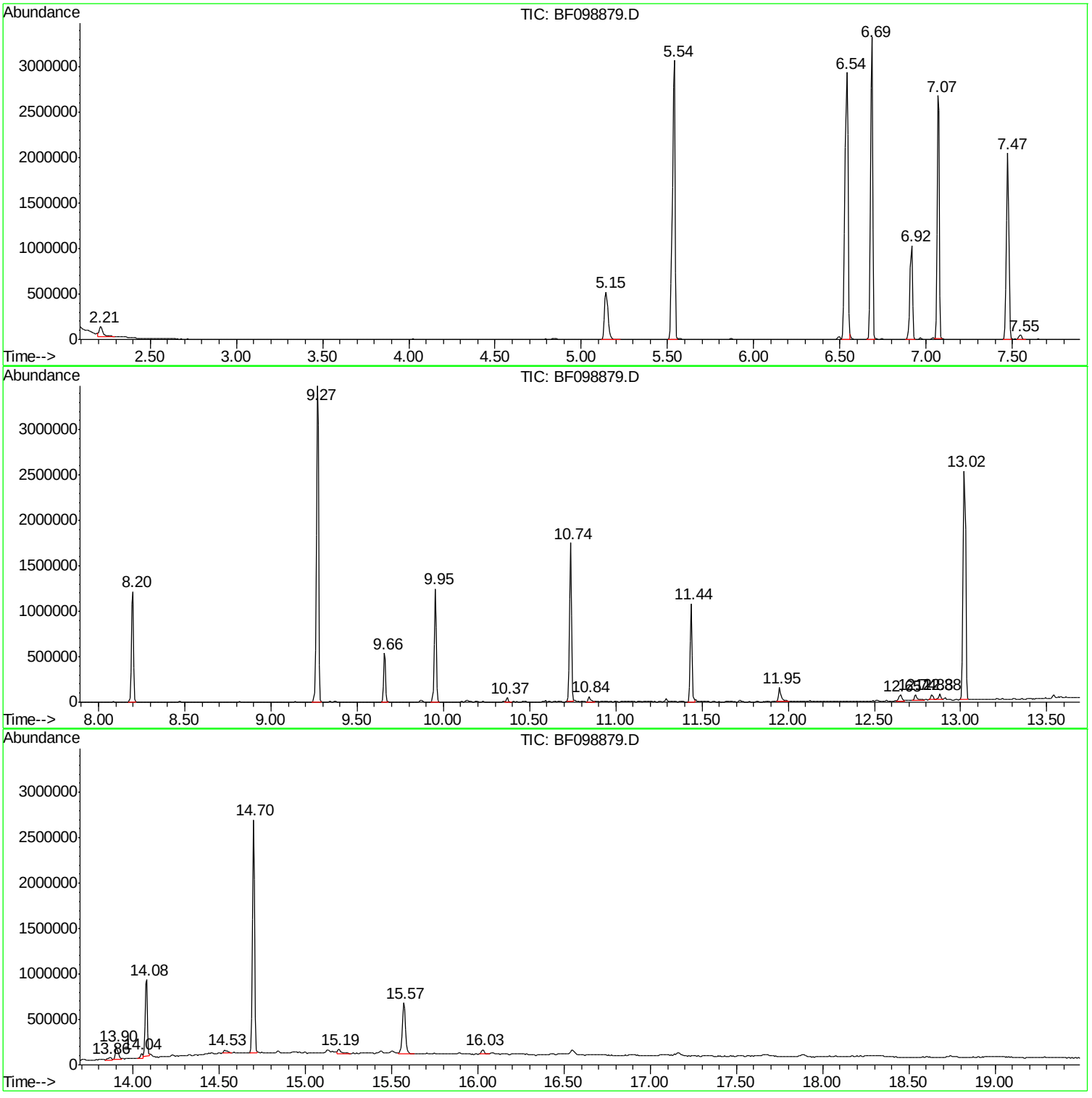
Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-116-2(5-10)

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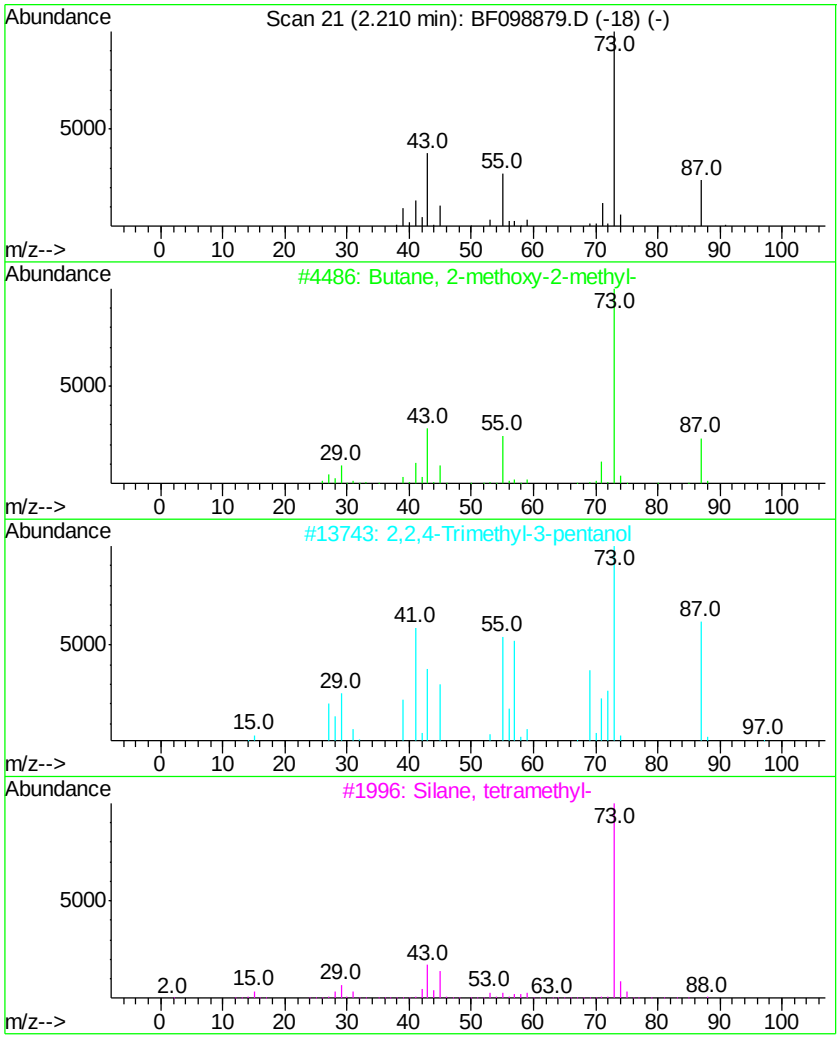
TIC Integration Parameters: LSCINT.P

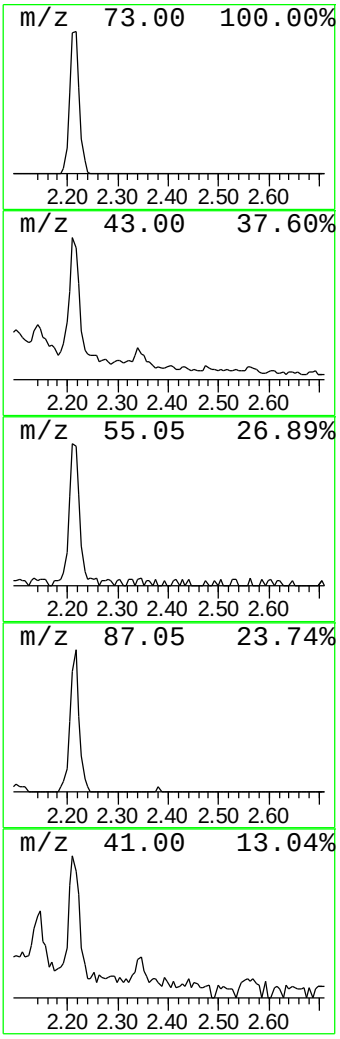
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	4.36 ng	198495	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	9





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Operator : SJ/JU
Sample : I5386-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-ENV-116-2(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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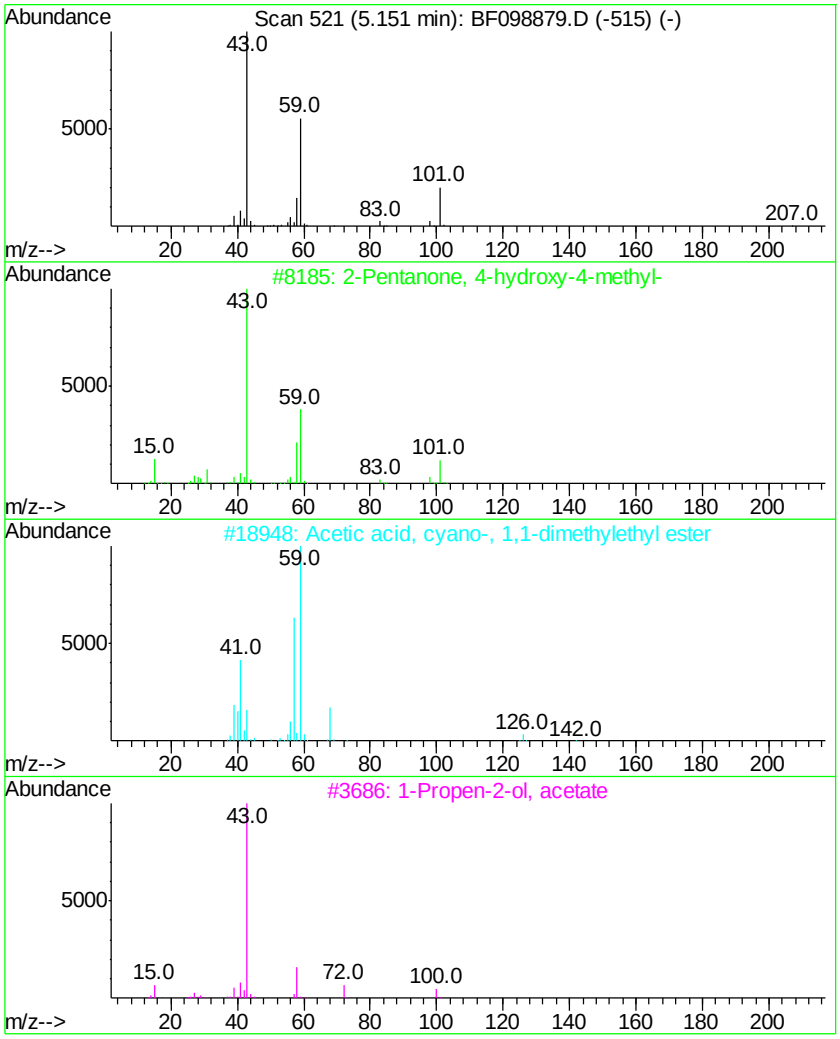
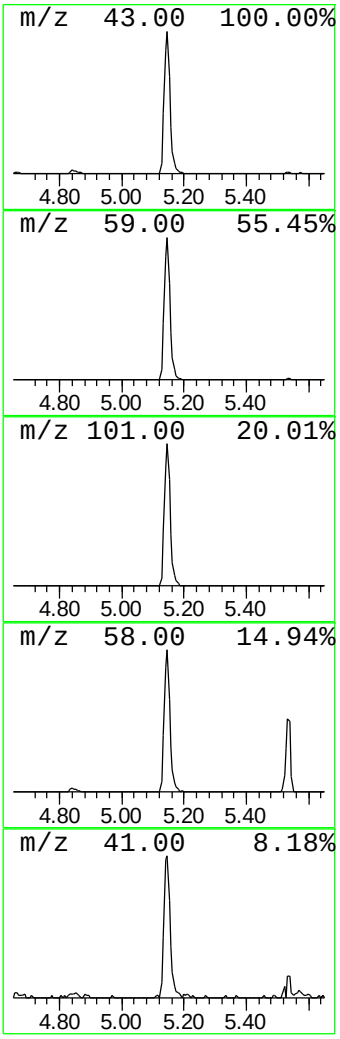
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	14.88 ng	677285	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SASP2P-ENV-116-2(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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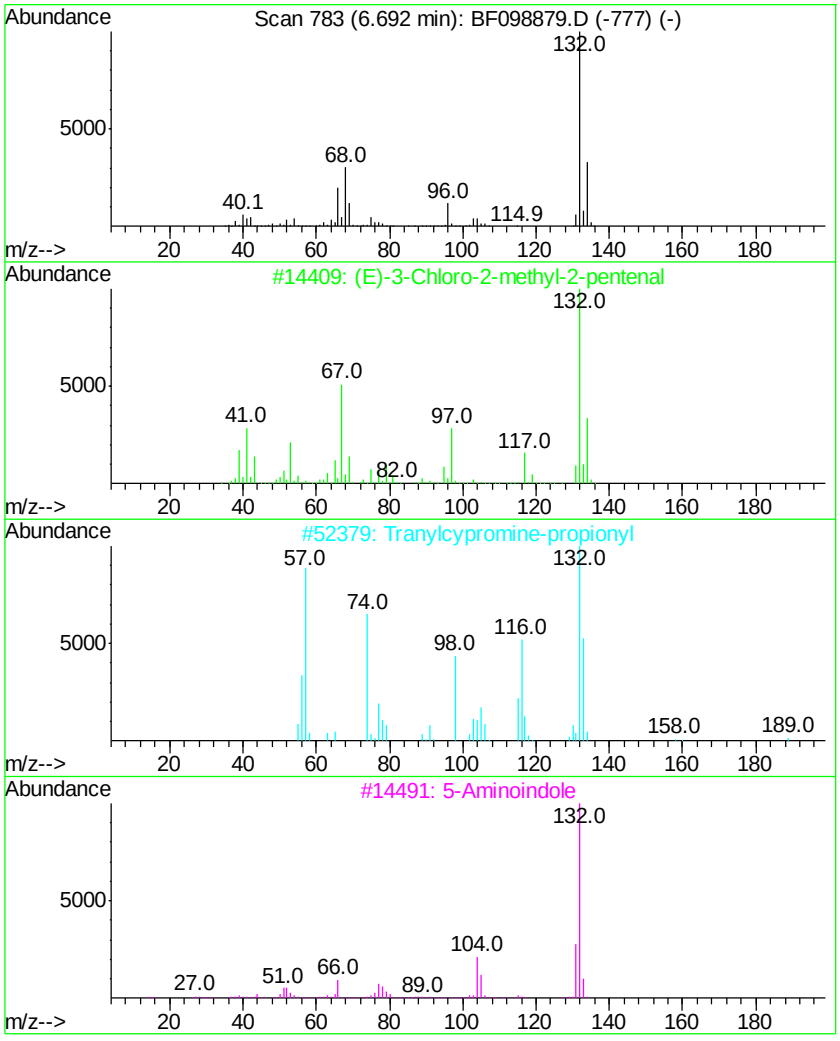
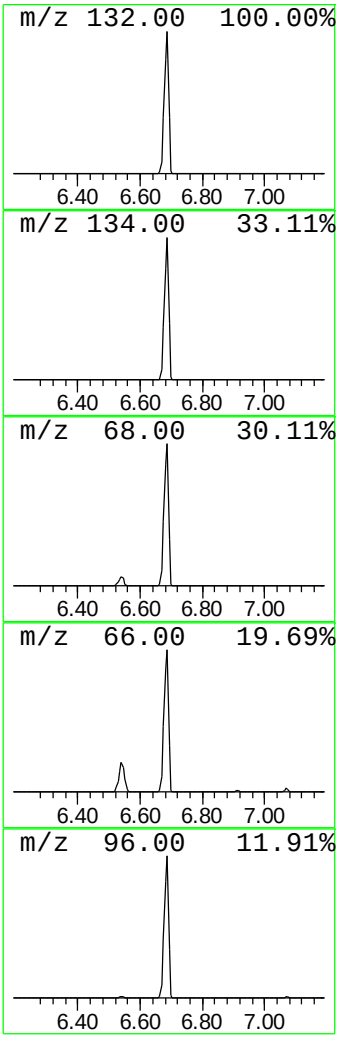
Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	70.62 ng	3214750	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Instrument :
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SASP2P-ENV-116-2(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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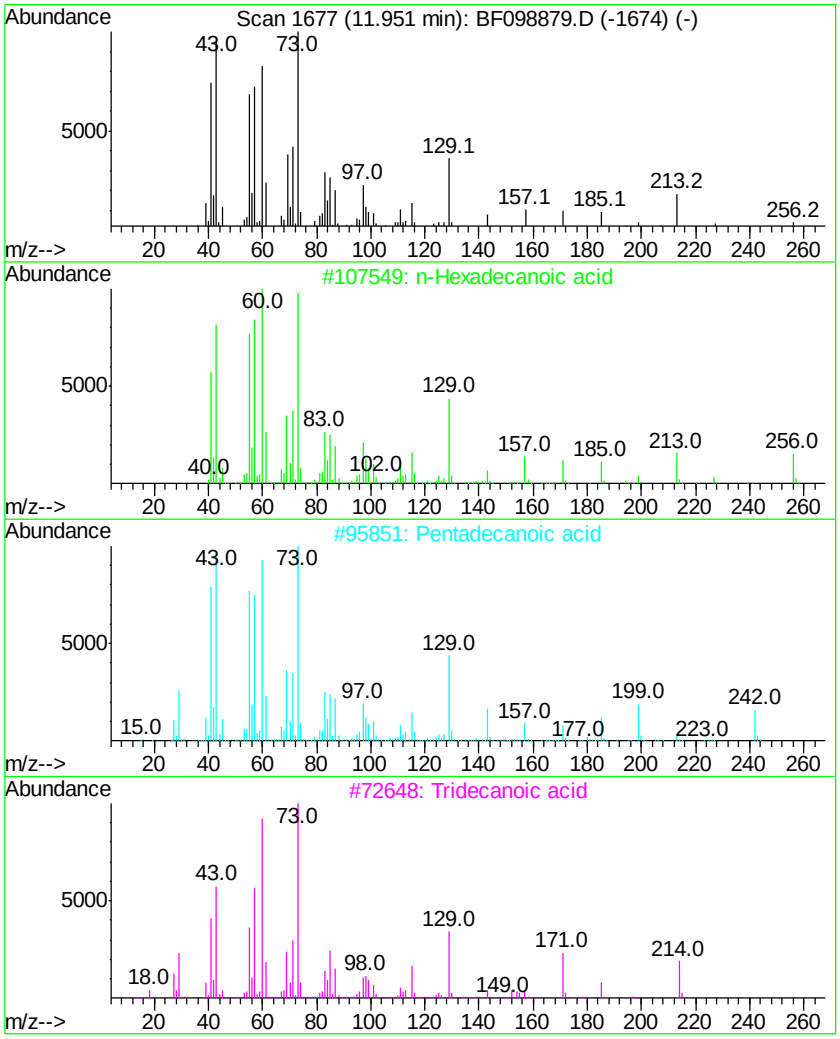
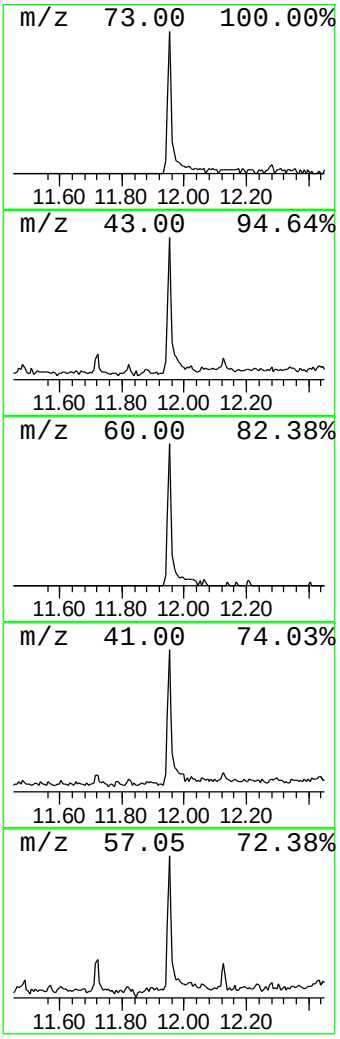
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	3.62 ng	160413	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20





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Instrument :
BNA_F
ClientSampleId :
SASP2P-ENV-116-2(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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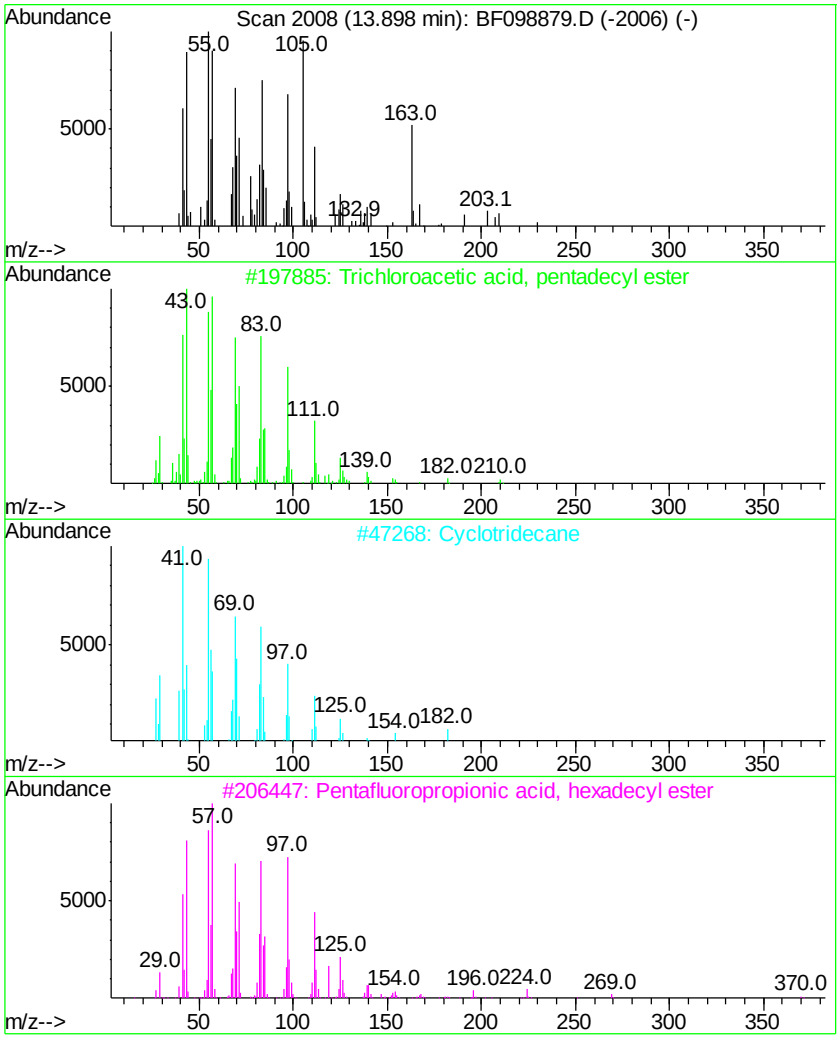
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

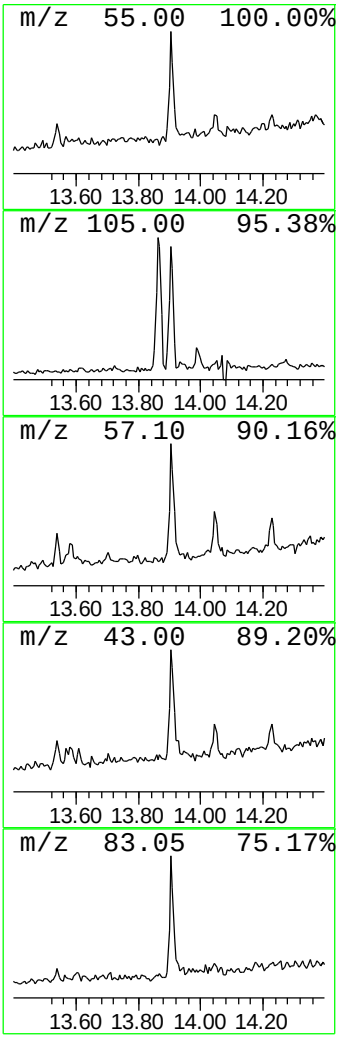
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	3.56 ng	146248	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2	Cyclotridecane	182	C13H26	000295-02-3	90
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	87
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	83
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	83





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Instrument : BNA_F
ClientSampleId : SASP2P-ENV-116-2(5-10)

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

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TIC Integration Parameters: LSCINT.P

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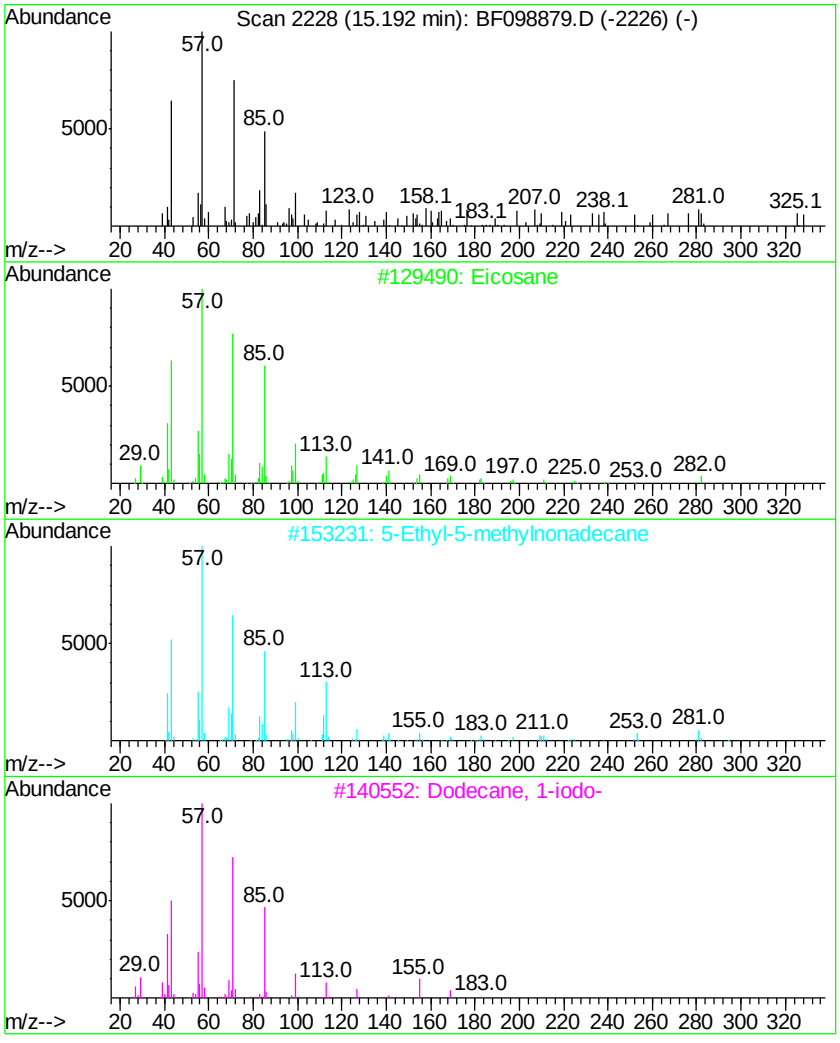
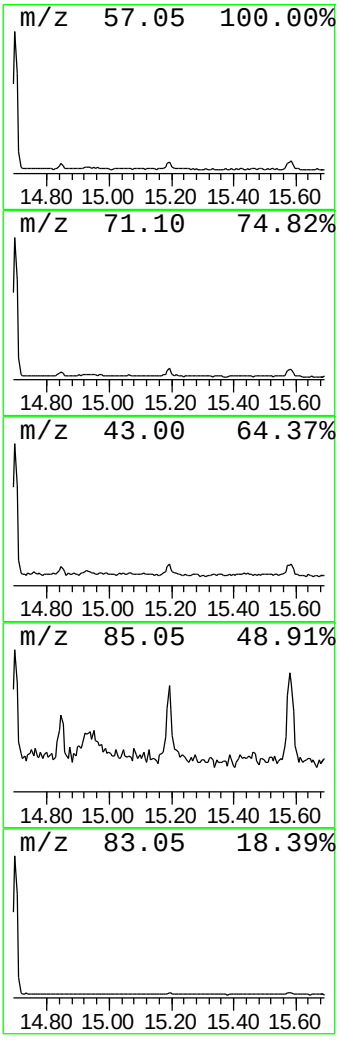
Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	2.14 ng	83213	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	68
2	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	64
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	59
4	Heptadecane	240	C17H36	000629-78-7	59
5	Docosane	310	C22H46	000629-97-0	59





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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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
Butane, 2-methoxy...	2.21	4.4	ng	198495	1	6.92	910475	20.0
2-Pentanone, 4-hy...	5.15	14.9	ng	677285	1	6.92	910475	20.0
unknown6.69	6.69	70.6	ng	3214750	1	6.92	910475	20.0
n-Hexadecanoic acid	11.95	3.6	ng	160413	4	11.44	885497	20.0
Trichloroacetic a...	13.90	3.6	ng	146248	5	14.08	820623	20.0
Eicosane	15.19	2.1	ng	83213	6	15.57	776678	20.0