LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\
Data File : BF095967.D
Acq On : 16 Jun 2017 21:22
Operator : SJ/MA
Sample : I3689-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BAYWAY-SWITCH-B

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-BF060517.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	4.516	493	498	516	rBV	43672	123217	7.82%	0.955%
2	5.216	614	617	649	rBV	553651	1284394	81.51%	9.952%
3	6.892	899	902	913	rBV	695455	1187454	75.36%	9.201%
4	6.981	913	917	937	rVB	934638	1575698	100.00%	12.209%
5	7.322	971	975	987	rVB	279009	372820	23.66%	2.889%
6	7.557	1010	1015	1026	rBV	764695	1014089	64.36%	7.858%
7	8.239	1127	1131	1151	rBV	526289	791992	50.26%	6.137%
8	9.351	1316	1320	1336	rBV	383558	547512	34.75%	4.242%
9	11.127	1617	1622	1640	rBV	1206039	1527385	96.93%	11.835%
10	11.827	1737	1741	1752	rBV	108555	138309	8.78%	1.072%
11	12.168	1795	1799	1805	rBV2	436582	554390	35.18%	4.296%
12	12.216	1805	1807	1812	rVB3	19048	23287	1.48%	0.180%
13	13.027	1939	1945	1949	rBV	22531	25119	1.59%	0.195%
14	13.468	2015	2020	2035	rBV	518350	788913	50.07%	6.113%
15	13.798	2071	2076	2081	rBV	19840	30175	1.92%	0.234%
16	14.562	2202	2206	2211	rBV2	380767	491464	31.19%	3.808%
17	14.604	2211	2213	2223	rVB	31599	47320	3.00%	0.367%
18	15.592	2377	2381	2386	rBV4	39540	51149	3.25%	0.396%
19	16.398	2514	2518	2524	rVB	51164	62979	4.00%	0.488%
20	16.698	2562	2569	2575	rBV	64658	95727	6.08%	0.742%
21	16.939	2606	2610	2617	rVB	927416	1006426	63.87%	7.798%
22	17.309	2669	2673	2678	rBV4	10029	16180	1.03%	0.125%
23	18.198	2818	2824	2835	rBV3	35059	68400	4.34%	0.530%
24	18.286	2835	2839	2845	rBV	308146	399171	25.33%	3.093%
25	19.568	3053	3057	3060	rBV	29073	39056	2.48%	0.303%
26	19.744	3084	3087	3093	rVB7	13388	21750	1.38%	0.169%
27	19.856	3102	3106	3112	rVB	17722	22363	1.42%	0.173%
28	19.909	3112	3115	3119	rBV	28327	32272	2.05%	0.250%
29	19.956	3119	3123	3135	rVV	292549	387959	24.62%	3.006%
30	20.391	3193	3197	3201	rBV3	14453	20474	1.30%	0.159%
31	20.444	3201	3206	3209	rBV7	9302	20096	1.28%	0.156%
32	21.168	3321	3329	3333	rBV7	16355	39982	2.54%	0.310%
33	21.268	3340	3346	3352	rBV6	30067	57189	3.63%	0.443%
34	21.491	3377	3384	3389	rBV5	19099	40902	2.60%	0.317%

LSC Area Percent Report

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Sample : I3689-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BAYWAY-SWITCH-B

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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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-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 12905613

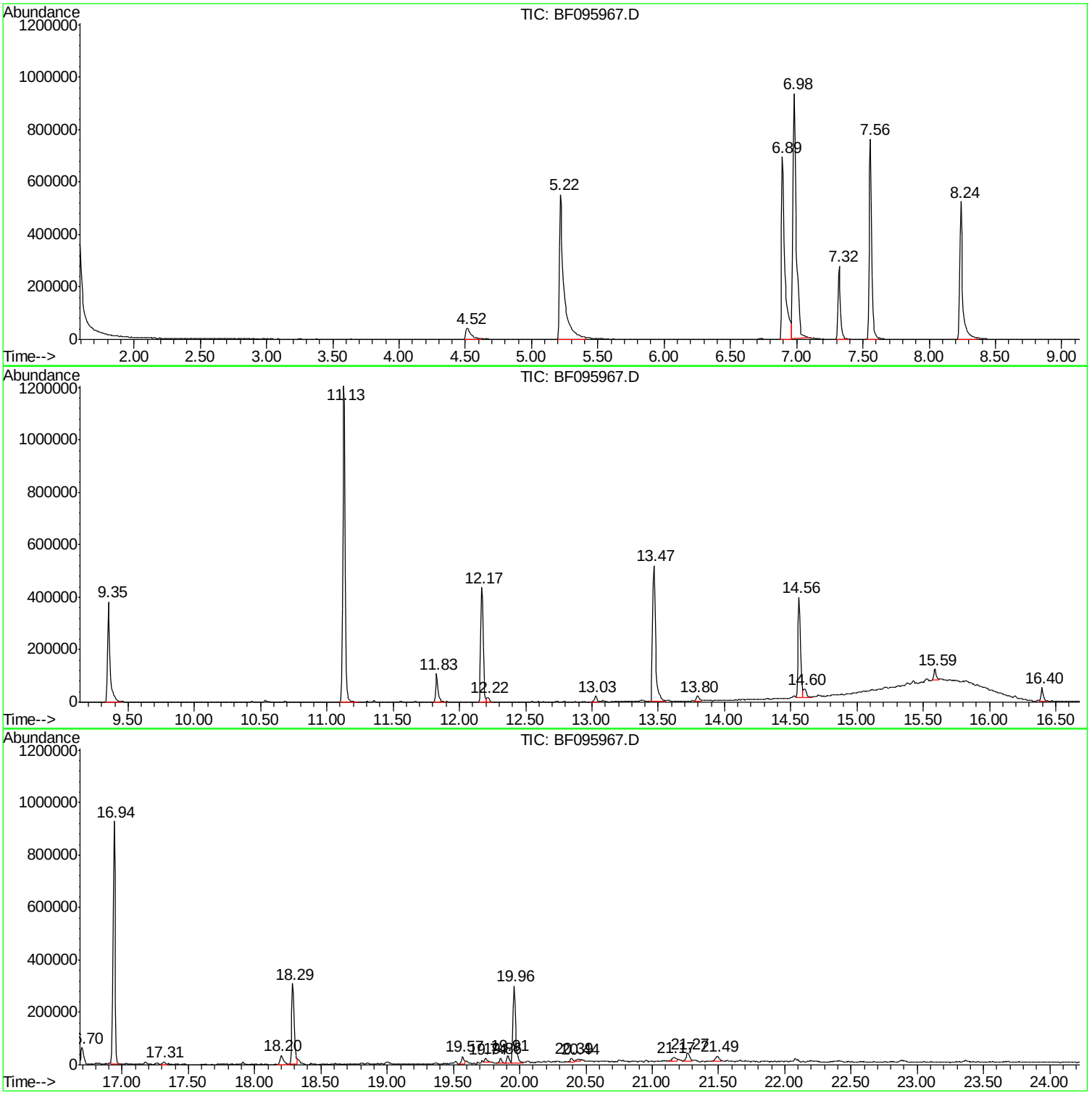
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\
Data File : BF095967.D
Acq On : 16 Jun 2017 21:22
Operator : SJ/MA
Sample : I3689-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BAYWAY-SWITCH-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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\BF061617\
Data File : BF095967.D
Acq On : 16 Jun 2017 21:22
Operator : SJ/MA
Sample : I3689-08
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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BAYWAY-SWITCH-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

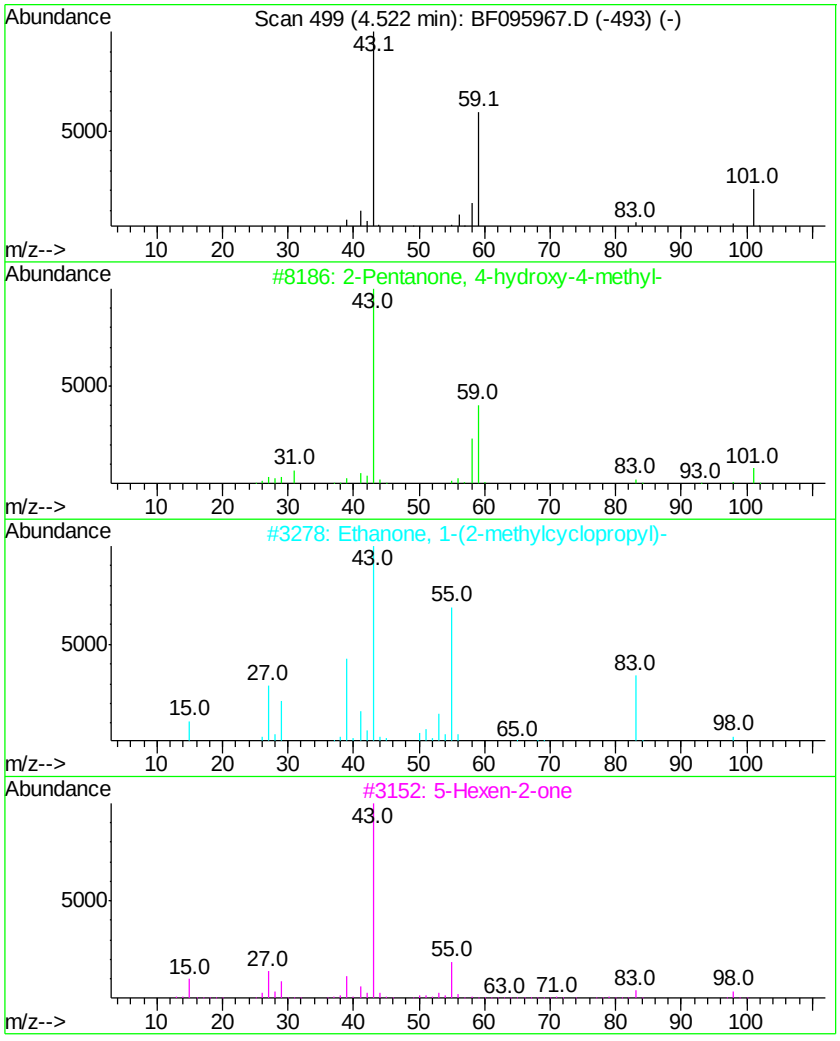
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

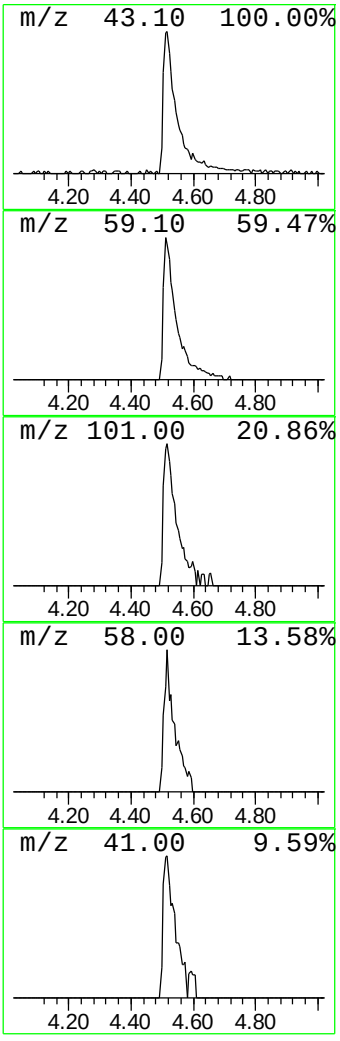
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	6.61 ng	123217	1,4-Dichlorobenzene-d4	7.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\
Data File : BF095967.D
Acq On : 16 Jun 2017 21:22
Operator : SJ/MA
Sample : I3689-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BAYWAY-SWITCH-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

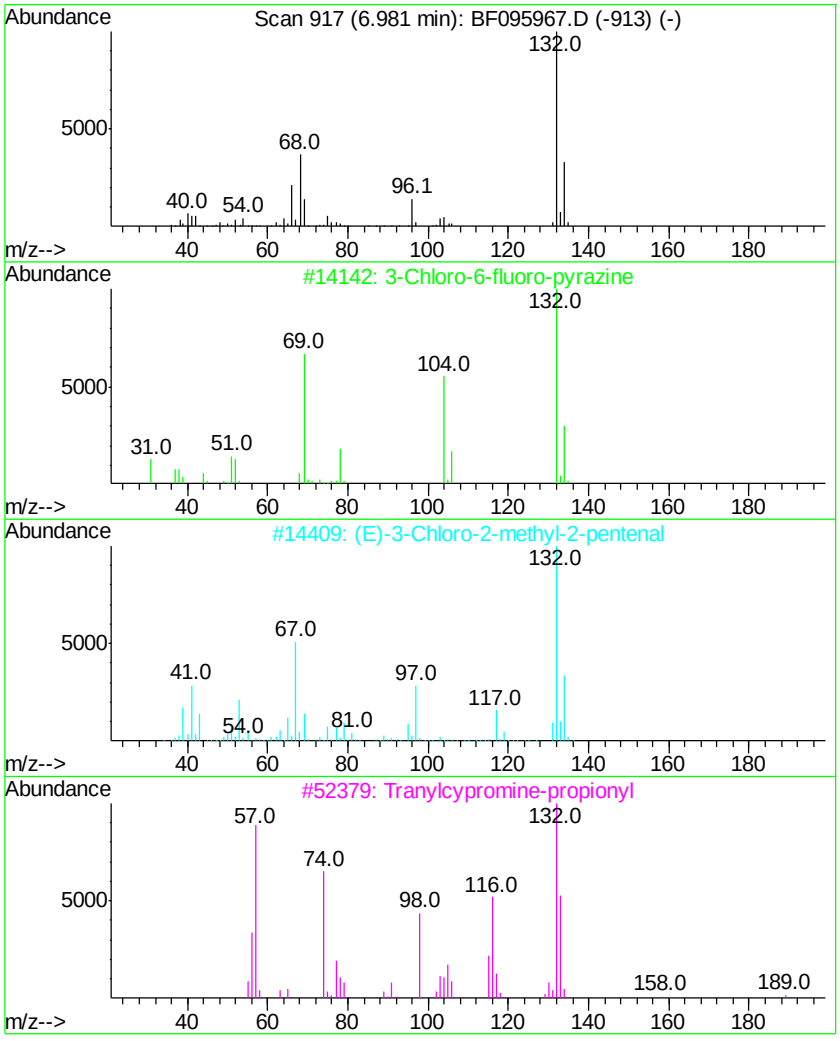
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

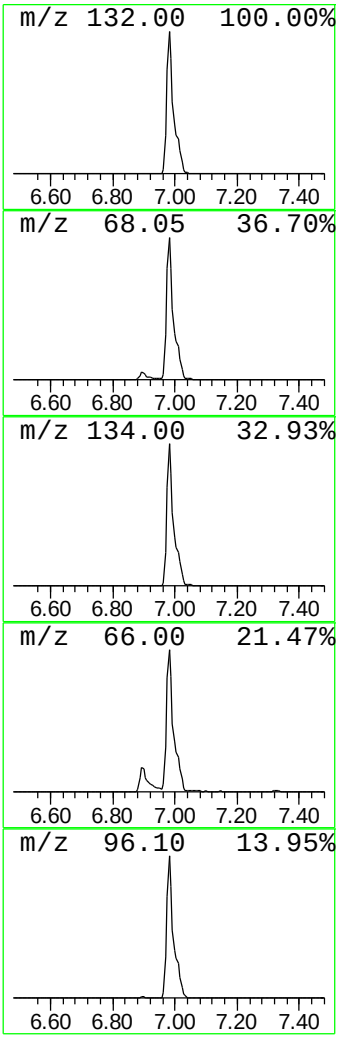
****

Peak Number 2 unknown6.98 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	84.53 ng	1575700	1,4-Dichlorobenzene-d4	7.32

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	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Benzeneethanamine, .alpha.-methy...	223	C16H17N	002980-02-1	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





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Operator : SJ/MA
Sample : I3689-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BAYWAY-SWITCH-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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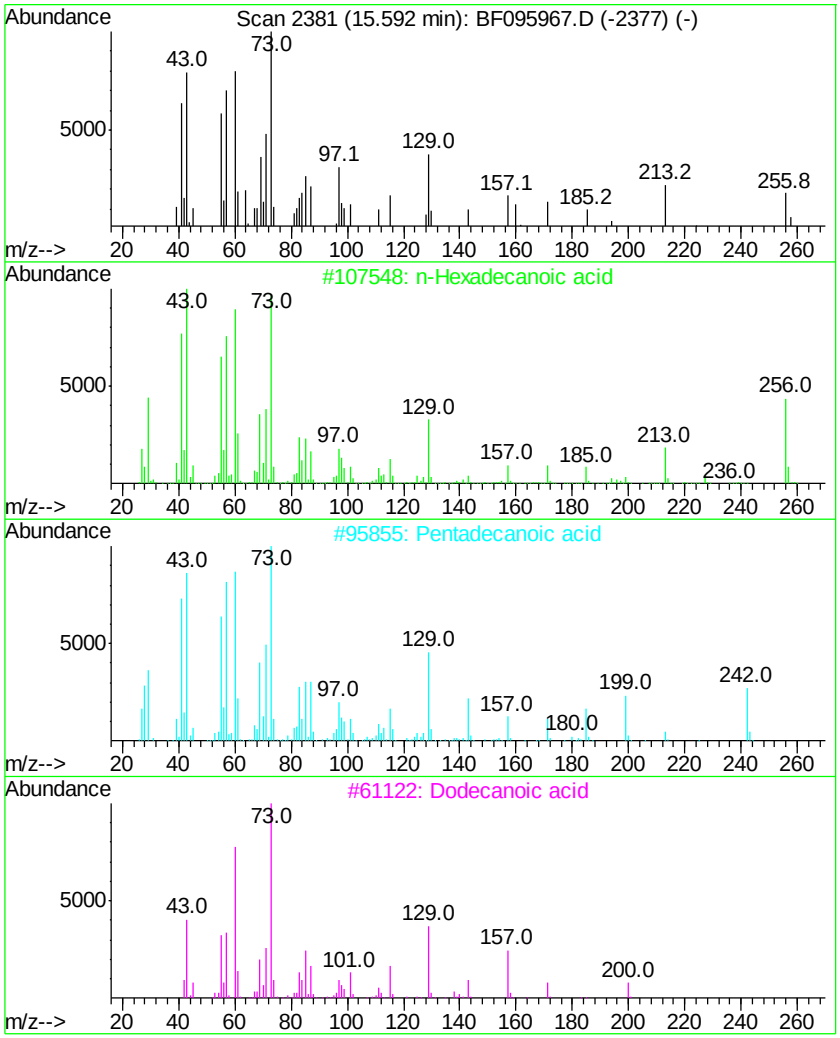
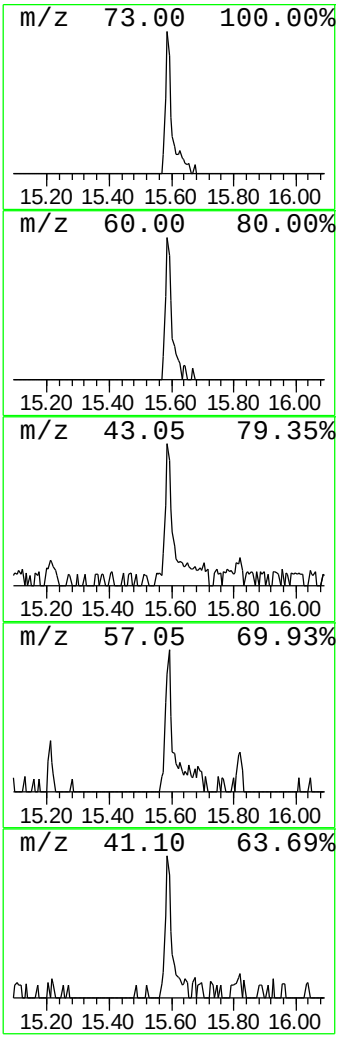
Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.59	2.08 ng	51149	Phenanthrene-d10	14.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Dodecanoic acid	200	C12H24O2	000143-07-7	58
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





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Sample : I3689-08
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Instrument : BNA_F
ClientSampleId : BAYWAY-SWITCH-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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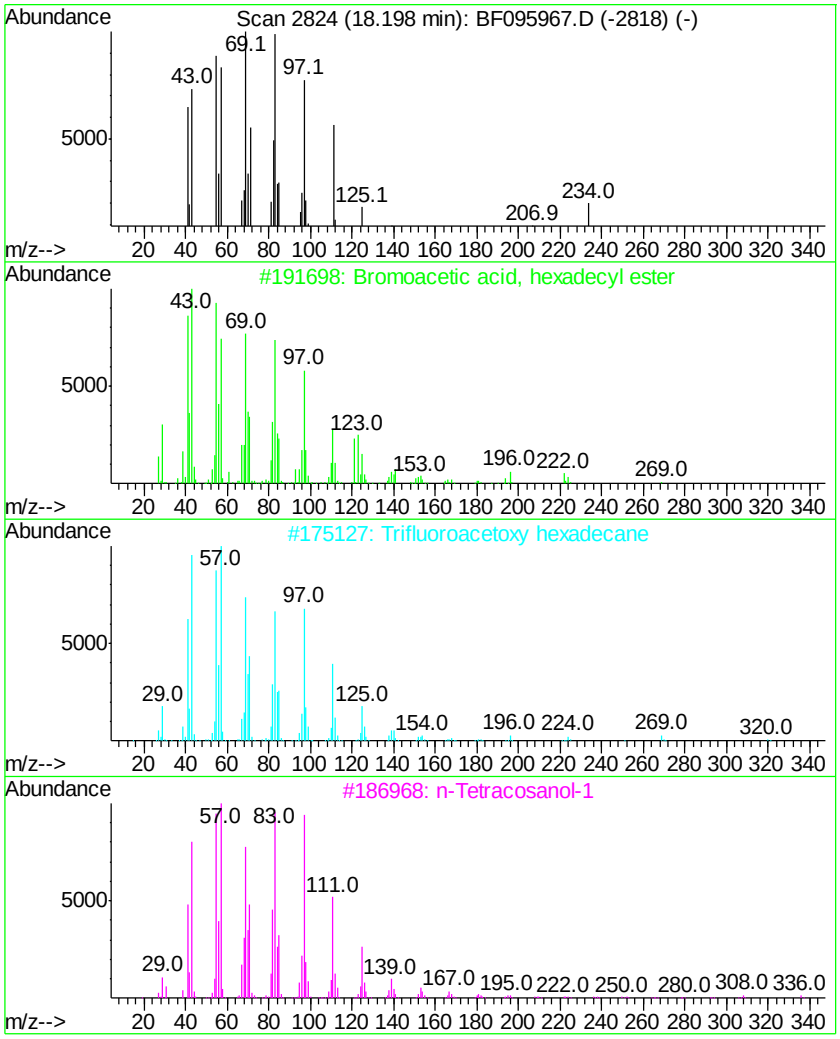
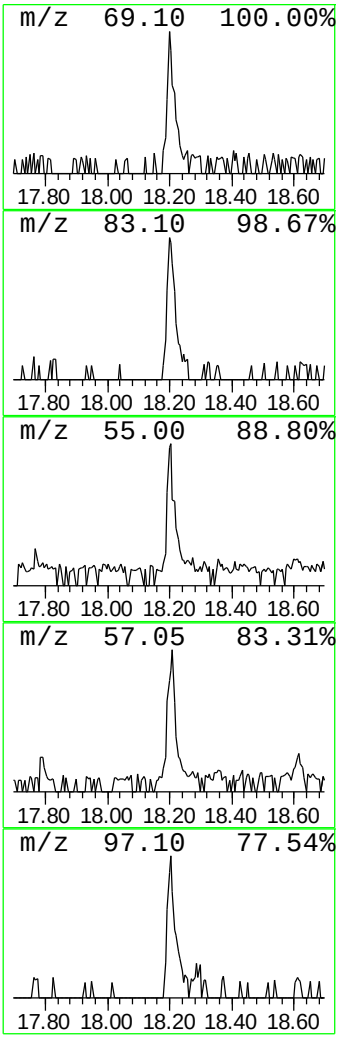
****

Peak Number 5 Bromoacetic acid, hexadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.20	3.43 ng	68400	Chrysene-d12	18.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	83
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	80
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	76
4	1-Heptacosanol	396	C27H56O	002004-39-9	76
5	1-Hexacosanol	382	C26H54O	000506-52-5	70





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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BAYWAY-SWITCH-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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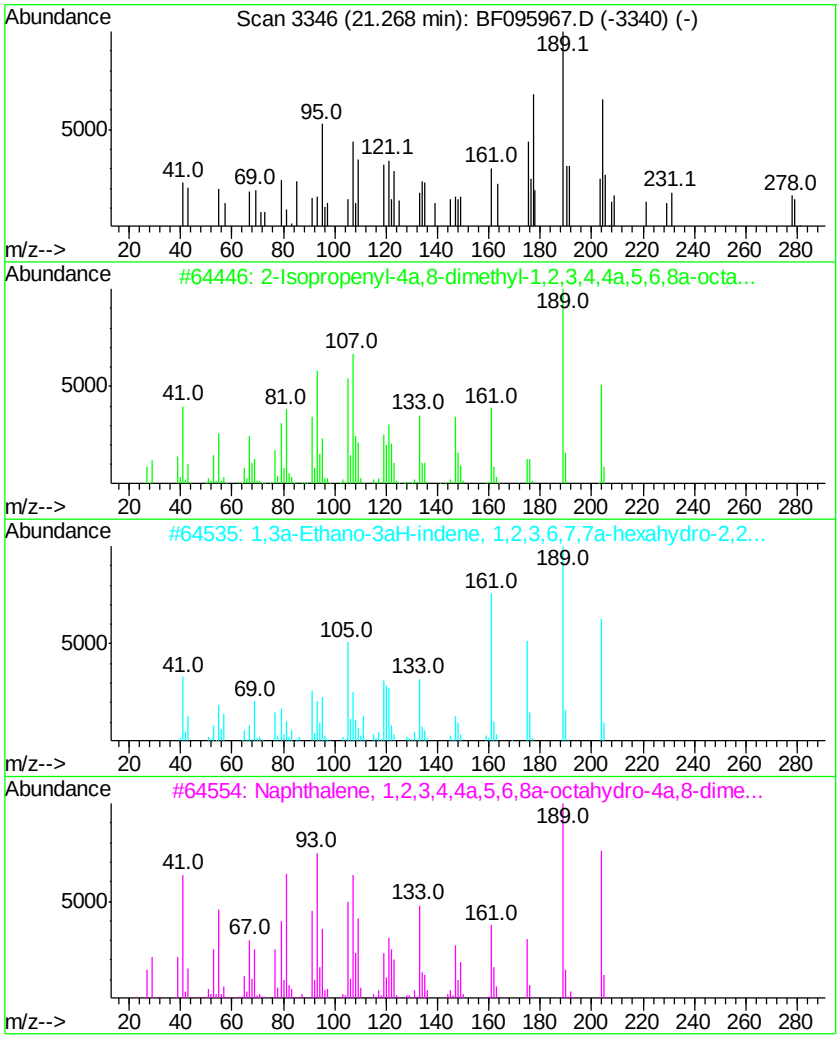
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

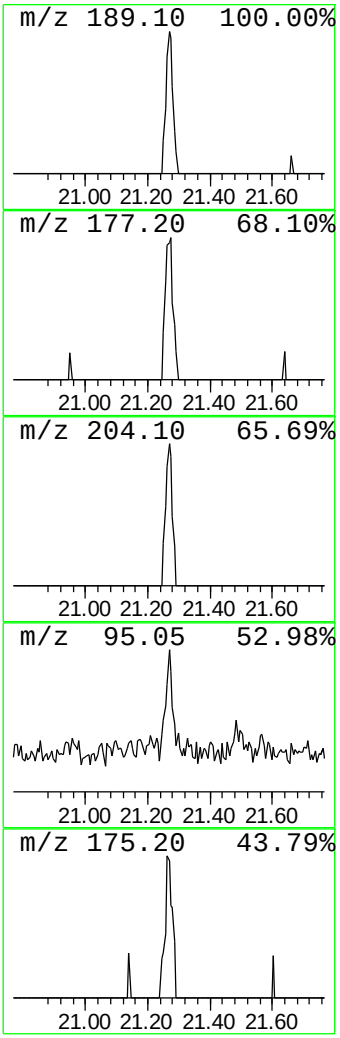
****

Peak Number 8 unknown21.27 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.27	2.95 ng	57189	Perylene-d12	19.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	45
2	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	43
3	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	38
4	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	30
5	Toluene, 4-chloro-2-fluoro-5-nitro-	189	C7H5ClFNO2	018349-11-6	27





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...	4.52	6.6	ng	123217	1	7.32	372820	20.0
unknown6.98	6.98	84.5	ng	1575700	1	7.32	372820	20.0
n-Hexadecanoic acid	15.59	2.1	ng	51149	4	14.56	491464	20.0
Bromoacetic acid,...	18.20	3.4	ng	68400	5	18.29	399171	20.0
unknown21.27	21.27	3.0	ng	57189	6	19.96	387959	20.0