LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096172.D
Acq On : 23 Jun 2017 22:03
Operator : SJ/MA
Sample : I3743-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FNDFL-VCTY-061517-COMP

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	1.540	7	9	39	rVB	643135	1170275	69.96%	7.532%
2	4.416	494	498	520	rBV	68044	212507	12.70%	1.368%
3	5.145	618	622	657	rBV	443538	1263511	75.53%	8.133%
4	6.839	906	910	920	rBV	517639	1072123	64.09%	6.901%
5	6.922	920	924	944	rVB	829540	1654037	98.88%	10.646%
6	7.257	977	981	993	rBV	271397	386165	23.09%	2.486%
7	7.492	1017	1021	1043	rBV	780433	1109918	66.35%	7.144%
8	8.181	1135	1138	1157	rBV	448735	788389	47.13%	5.074%
9	9.292	1323	1327	1352	rBV	342865	536881	32.10%	3.456%
10	11.074	1624	1630	1651	rBV	1315945	1672756	100.00%	10.767%
11	11.774	1745	1749	1762	rBV	103465	151372	9.05%	0.974%
12	11.904	1767	1771	1777	rVB	15423	20814	1.24%	0.134%
13	12.110	1802	1806	1812	rBV2	430951	566499	33.87%	3.646%
14	12.163	1812	1815	1821	rVB3	15535	27852	1.67%	0.179%
15	12.968	1948	1952	1958	rBB2	13102	16951	1.01%	0.109%
16	13.410	2023	2027	2052	rBB	510081	806927	48.24%	5.194%
17	13.739	2078	2083	2091	rBV	17661	29626	1.77%	0.191%
18	14.504	2209	2213	2218	rBV	376200	506673	30.29%	3.261%
19	14.545	2218	2220	2232	rVB	53148	86496	5.17%	0.557%
20	14.651	2232	2238	2245	rBV	15336	25573	1.53%	0.165%
21	15.474	2368	2378	2383	rBV5	12018	29387	1.76%	0.189%
22	15.539	2385	2389	2395	rVV2	58412	73824	4.41%	0.475%
23	16.345	2520	2526	2536	rVB	115761	151165	9.04%	0.973%
24	16.645	2573	2577	2586	rBV	135805	179770	10.75%	1.157%
25	16.892	2615	2619	2626	rVB	994954	1192851	71.31%	7.678%
26	17.127	2656	2659	2665	rVB2	18538	24461	1.46%	0.157%
27	17.215	2669	2674	2677	rBV2	15600	20193	1.21%	0.130%
28	17.262	2678	2682	2687	rBV4	16693	25822	1.54%	0.166%
29	18.150	2829	2833	2843	rBV	79323	124589	7.45%	0.802%
30	18.245	2844	2849	2853	rBV2	386263	516321	30.87%	3.323%
31	18.286	2853	2856	2859	rVB	34821	46307	2.77%	0.298%
32	18.762	2934	2937	2942	rVB3	17294	19535	1.17%	0.126%
33	19.392	3041	3044	3048	rVB5	25772	30088	1.80%	0.194%
34	19.521	3062	3066	3069	rBV	95318	122874	7.35%	0.791%

LSC Area Percent Report

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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FNDFL-VCTY-061517-COMP

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

35	19.639	3083	3086	3089	rBV2	26072	29974	1.79%	0.193%
36	19.680	3090	3093	3095	rBV3	14948	18420	1.10%	0.119%
37	19.815	3112	3116	3120	rBV	63024	77854	4.65%	0.501%
38	19.874	3122	3126	3130	rVV	81757	94073	5.62%	0.605%
39	19.921	3130	3134	3145	rBV	316825	462668	27.66%	2.978%
40	20.350	3205	3207	3210	rVB4	23169	24587	1.47%	0.158%
41	21.097	3330	3334	3337	rBV2	29914	47258	2.83%	0.304%
42	21.427	3385	3390	3396	rVB2	40181	83650	5.00%	0.538%
43	22.133	3505	3510	3511	rBV5	10287	18020	1.08%	0.116%
44	22.803	3622	3624	3630	rVB7	13123	17518	1.05%	0.113%

Sum of corrected areas: 15536554

LSC Report - Integrated Chromatogram

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Data File : BF096172.D
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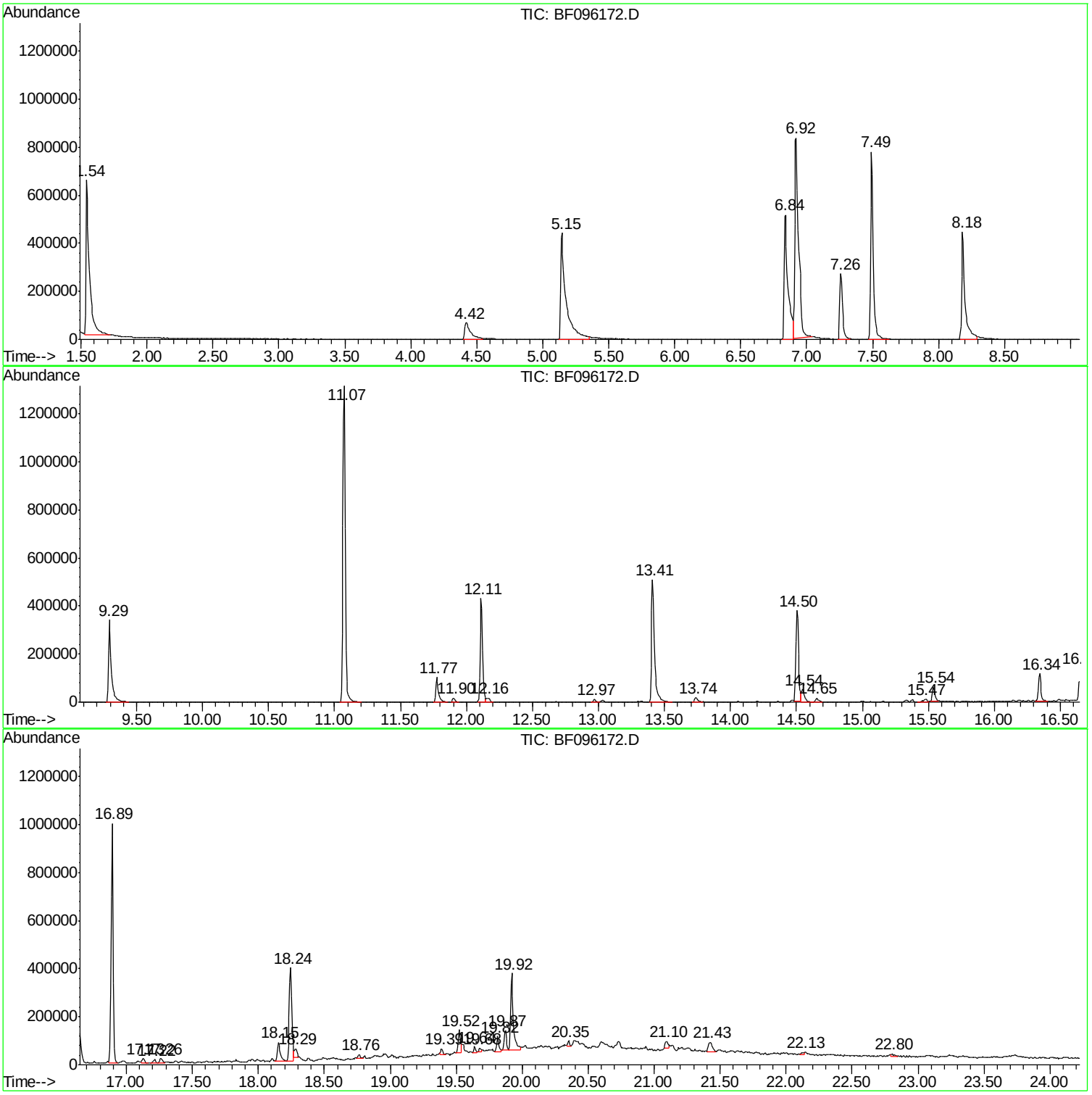
Operator : SJ/MA
Sample : I3743-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FNDFL-VCTY-061517-COMP

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\BF062317\
Data File : BF096172.D
Acq On : 23 Jun 2017 22:03
Operator : SJ/MA
Sample : I3743-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FNDFL-VCTY-061517-COMP

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

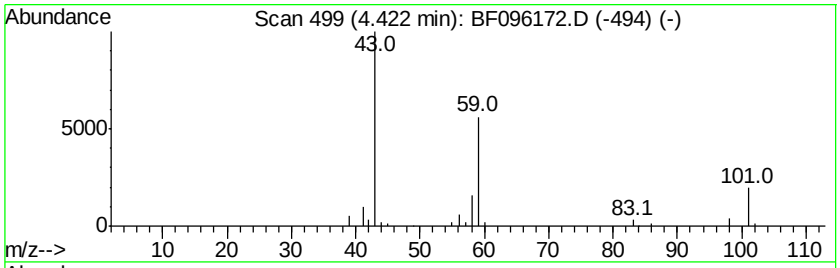
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

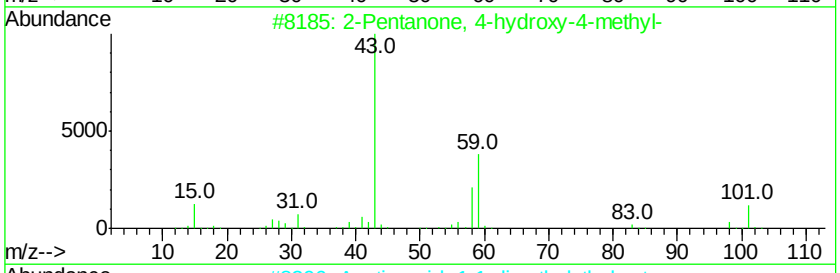
****

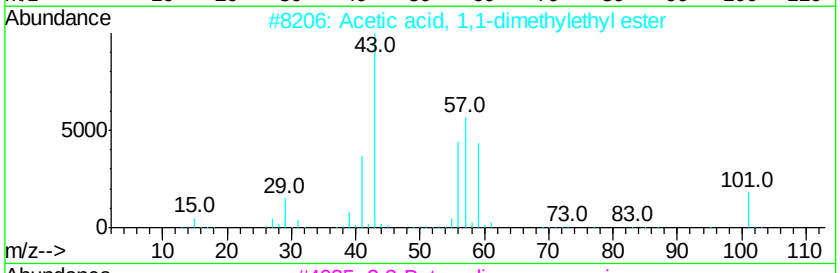
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

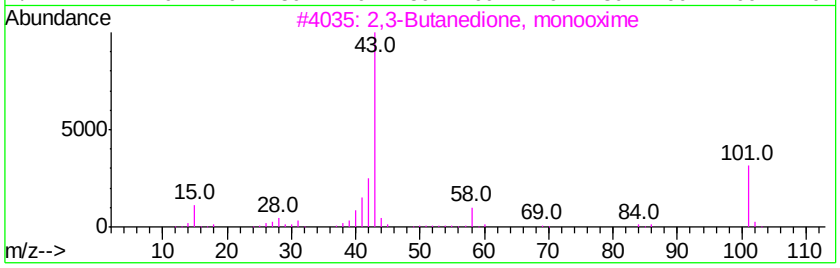
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.42	11.01 ng	212507	1,4-Dichlorobenzene-d4	7.26

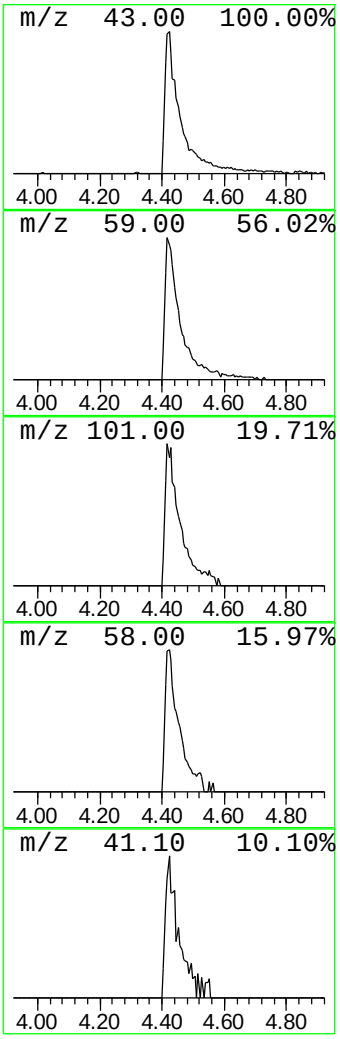
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
4	3-Hexanol	102	C6H14O	000623-37-0	28
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25











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Data File : BF096172.D
Acq On : 23 Jun 2017 22:03
Operator : SJ/MA
Sample : I3743-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FNDFL-VCTY-061517-COMP

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

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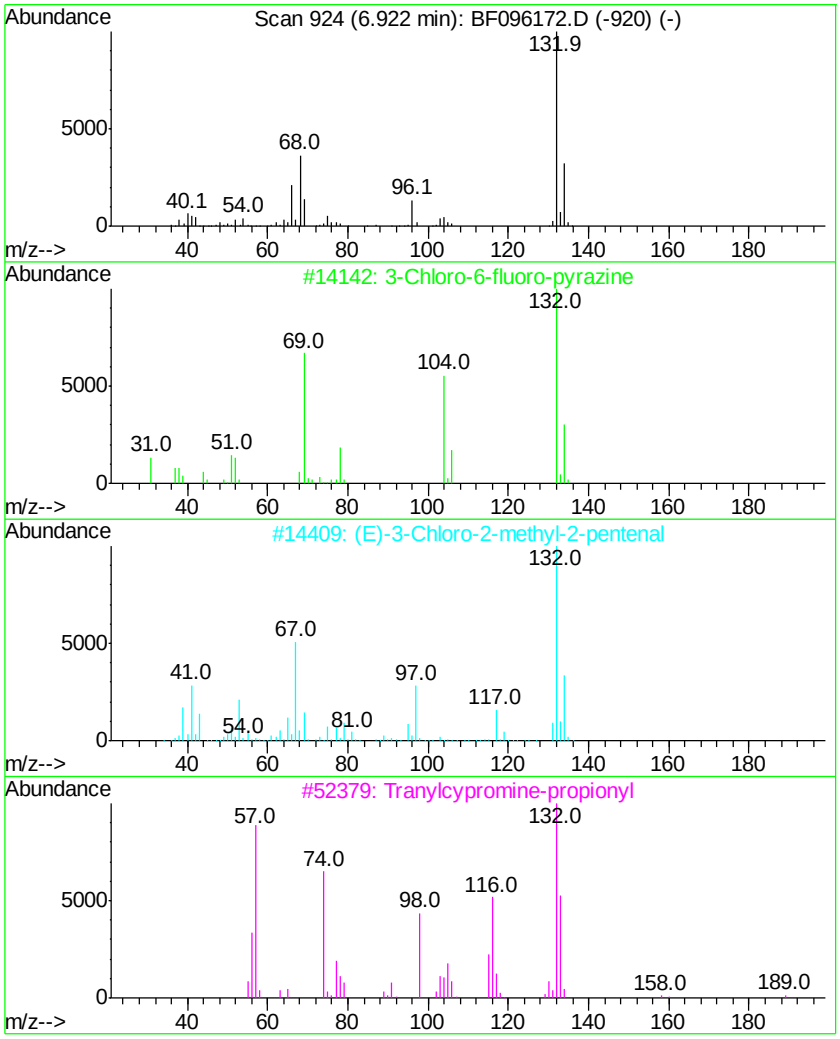
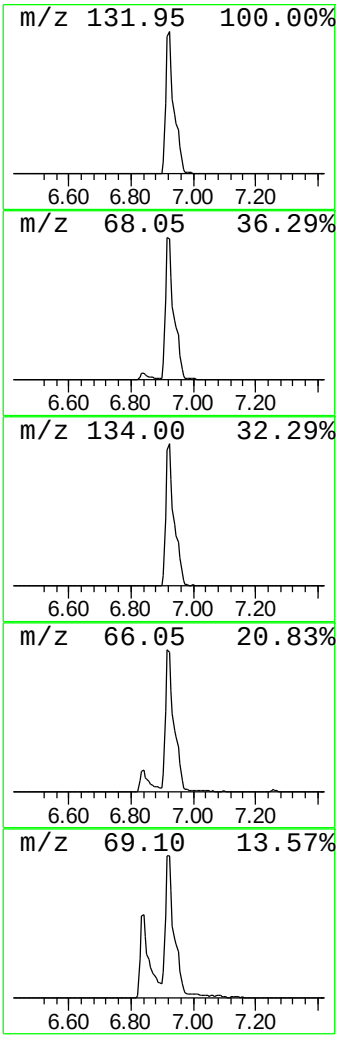
Peak Number 3 unknown6.92 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.92	85.66 ng	1654040	1,4-Dichlorobenzene-d4	7.26

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	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Xenon	132	Xe	007440-63-3	9
5	1-Aminoindan	133	C9H11N	034698-41-4	9





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Operator : SJ/MA
Sample : I3743-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FNDFL-VCTY-061517-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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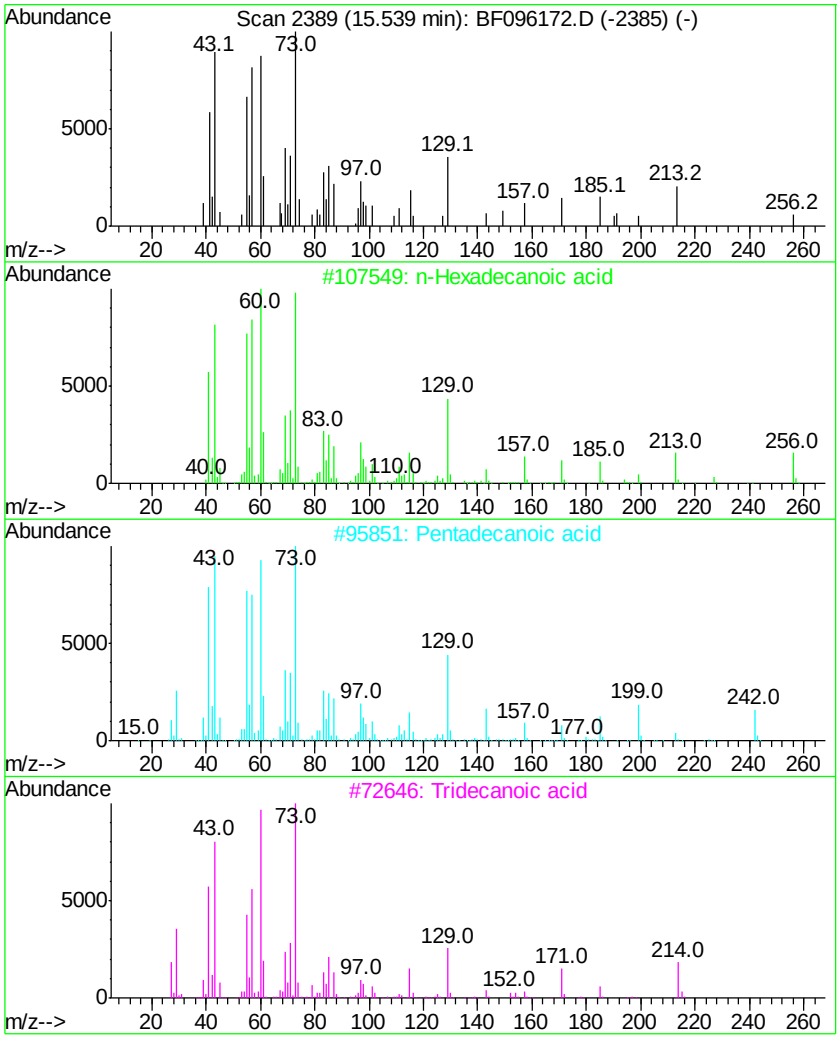
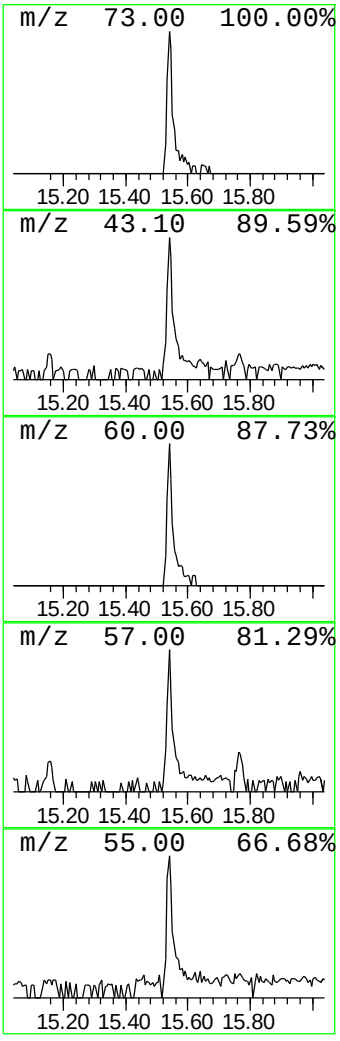
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	2.91 ng	73824	Phenanthrene-d10	14.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : FNDFL-VCTY-061517-COMP

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

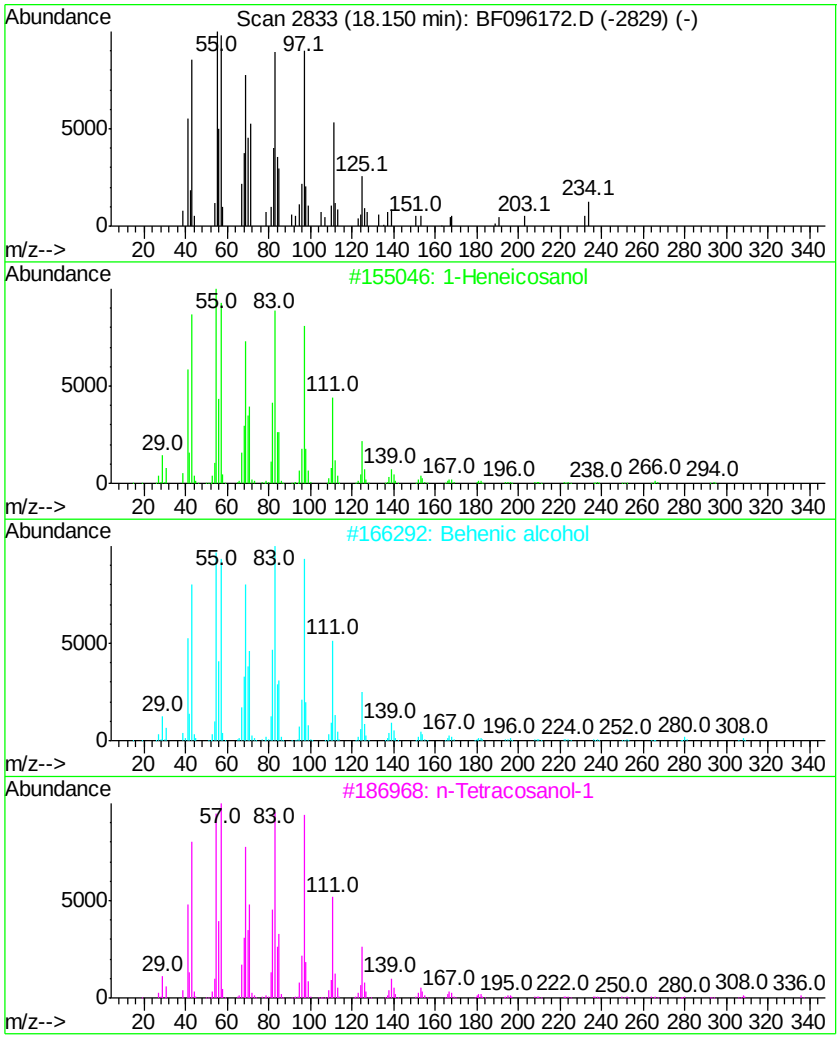
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

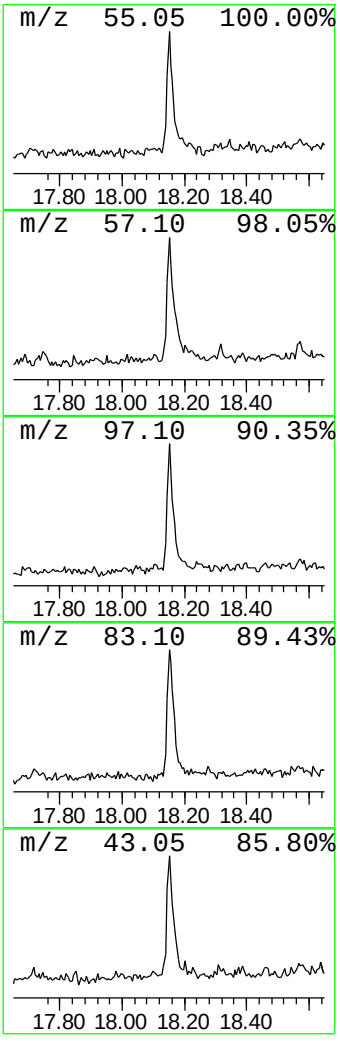
****

Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.15	4.83 ng	124589	Chrysene-d12	18.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	1-Heptacosanol	396	C27H56O	002004-39-9	95
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94





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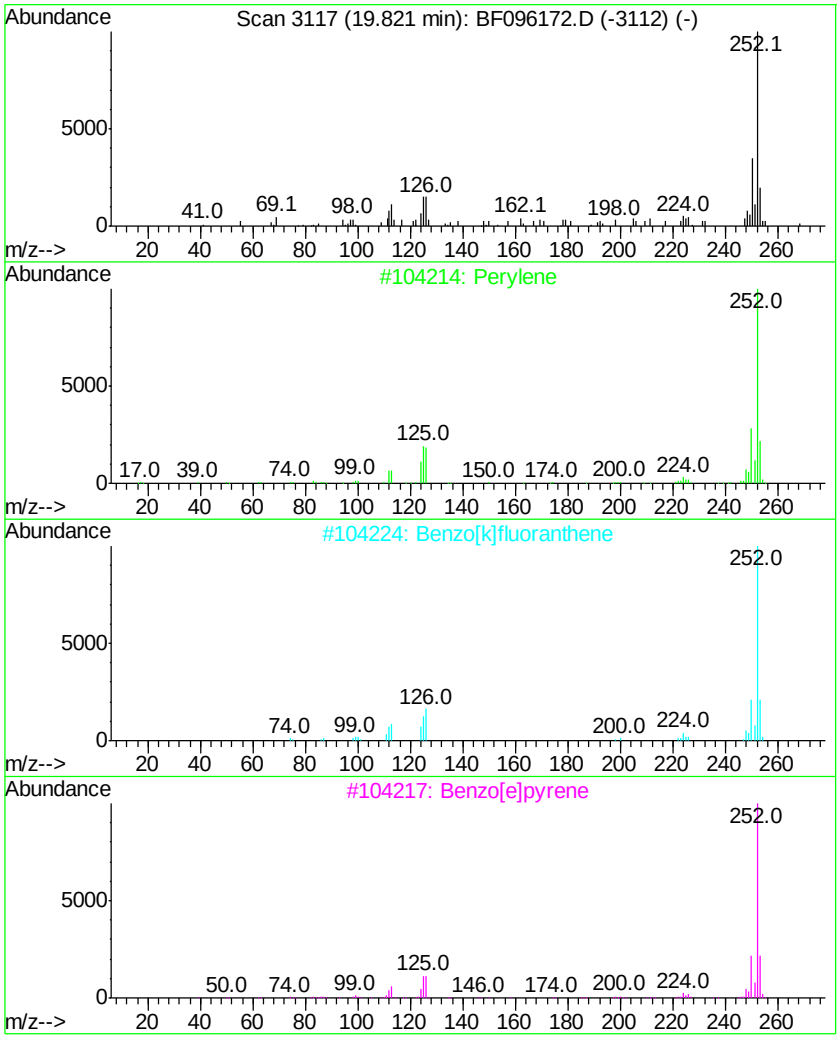
TIC Integration Parameters: LSCINT.P

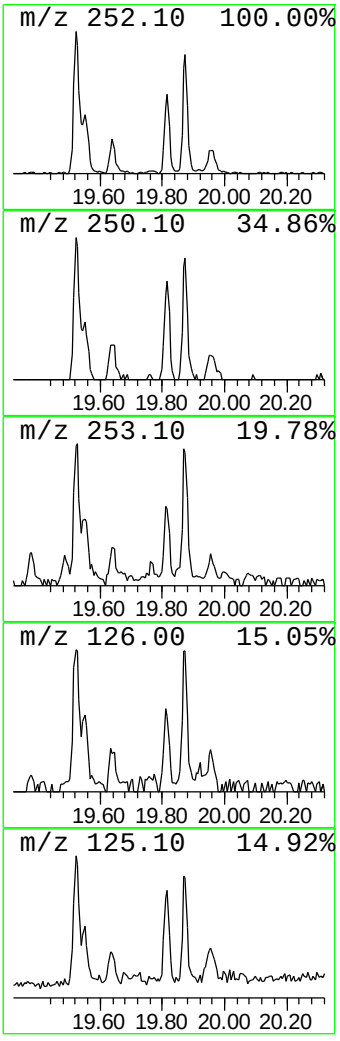
****

Peak Number 7 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.82	3.37 ng	77854	Perylene-d12	19.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	97
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benzo[e]pyrene	252	C20H12	000192-97-2	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	87





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...	4.42	11.0	ng	212507	1	7.26	386165	20.0
unknown6.92	6.92	85.7	ng	1654040	1	7.26	386165	20.0
n-Hexadecanoic acid	15.54	2.9	ng	73824	4	14.50	506673	20.0
1-Heneicosanol	18.15	4.8	ng	124589	5	18.24	516321	20.0
Perylene	19.82	3.4	ng	77854	6	19.92	462668	20.0