LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095282.D
Acq On : 20 May 2017 1:23
Operator : SJ/MA
Sample : I3202-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2COMP

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-BF050217.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	5.107	535	539	563	rBV	203961	568551	22.35%	2.545%
2	5.725	641	644	675	rBV	933626	2086925	82.05%	9.342%
3	6.307	739	743	752	rBV2	15481	30837	1.21%	0.138%
4	7.301	908	912	929	rBV	1196515	2049573	80.58%	9.175%
5	7.425	929	933	945	rVB	1573088	2434501	95.72%	10.898%
6	7.760	987	990	1005	rBV	447954	558015	21.94%	2.498%
7	7.995	1026	1030	1047	rBV	1415362	1803295	70.90%	8.072%
8	8.660	1139	1143	1176	rBV	792775	1370689	53.89%	6.136%
9	9.783	1329	1334	1358	rBV	387229	687768	27.04%	3.079%
10	10.966	1529	1535	1543	rBV2	19541	34817	1.37%	0.156%
11	11.107	1555	1559	1567	rBV	22858	39203	1.54%	0.175%
12	11.548	1629	1634	1649	rBV	1813875	2543419	100.00%	11.385%
13	12.095	1720	1727	1731	rBV5	19859	40144	1.58%	0.180%
14	12.136	1731	1734	1741	rVB2	19915	27706	1.09%	0.124%
15	12.248	1749	1753	1765	rBV	168689	312337	12.28%	1.398%
16	12.613	1810	1815	1822	rBV2	531740	780269	30.68%	3.493%
17	12.665	1822	1824	1832	rVB2	27478	44459	1.75%	0.199%
18	12.989	1871	1879	1887	rBV4	15966	35633	1.40%	0.160%
19	13.442	1951	1956	1962	rBV	43149	51705	2.03%	0.231%
20	13.524	1962	1970	1977	rBV2	26793	49349	1.94%	0.221%
21	13.807	2009	2018	2022	rBV5	17206	37298	1.47%	0.167%
22	13.907	2030	2035	2056	rBV	750925	1231147	48.41%	5.511%
23	14.218	2083	2088	2090	rBV2	55678	64436	2.53%	0.288%
24	14.242	2090	2092	2099	rVB4	20893	30992	1.22%	0.139%
25	14.948	2207	2212	2216	rBV	33314	39479	1.55%	0.177%
26	15.018	2216	2224	2228	rVV2	409814	618431	24.31%	2.768%
27	15.054	2228	2230	2239	rVV	129345	199563	7.85%	0.893%
28	15.154	2243	2247	2256	rVB	24585	49724	1.96%	0.223%
29	15.548	2310	2314	2320	rVB6	14436	27035	1.06%	0.121%
30	15.759	2345	2350	2355	rBV	44331	51168	2.01%	0.229%
31	15.806	2355	2358	2362	rVV	33113	42223	1.66%	0.189%
32	15.848	2362	2365	2372	rVB	34698	48324	1.90%	0.216%
33	15.954	2379	2383	2389	rBV3	49307	116806	4.59%	0.523%
34	16.595	2488	2492	2496	rBV	38471	49869	1.96%	0.223%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095282.D
Acq On : 20 May 2017 1:23
Operator : SJ/MA
Sample : I3202-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2COMP

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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.642	2496	2500	2503	rVV4	19744	29584	1.16%	0.132%
36	16.718	2509	2513	2515	rVV2	91290	101579	3.99%	0.455%
37	16.748	2515	2518	2522	rVV	132481	147067	5.78%	0.658%
38	16.801	2523	2527	2537	rVB	169325	222687	8.76%	0.997%
39	16.877	2537	2540	2543	rBV3	23732	28080	1.10%	0.126%
40	17.100	2574	2578	2584	rBV	212951	272107	10.70%	1.218%
41	17.330	2613	2617	2626	rBV	1237472	1496294	58.83%	6.698%
42	17.412	2628	2631	2638	rVB8	18496	35353	1.39%	0.158%
43	17.565	2654	2657	2663	rVB2	34609	49138	1.93%	0.220%
44	17.653	2663	2672	2676	rBV2	35862	58053	2.28%	0.260%
45	17.700	2676	2680	2689	rBV3	39107	79887	3.14%	0.358%
46	17.812	2697	2699	2703	rBV	30196	37809	1.49%	0.169%
47	18.577	2826	2829	2834	rBV5	34715	72905	2.87%	0.326%
48	18.683	2843	2847	2852	rBV2	417000	631427	24.83%	2.826%
49	19.318	2952	2955	2956	rBV3	36526	34999	1.38%	0.157%
50	19.965	3061	3065	3068	rBV	88956	137461	5.40%	0.615%
51	20.253	3111	3114	3118	rVB	84617	93409	3.67%	0.418%
52	20.312	3121	3124	3129	rVV	101121	138346	5.44%	0.619%
53	20.365	3129	3133	3142	rVB	330236	456168	17.94%	2.042%
54	20.824	3208	3211	3214	rBV3	49670	61800	2.43%	0.277%

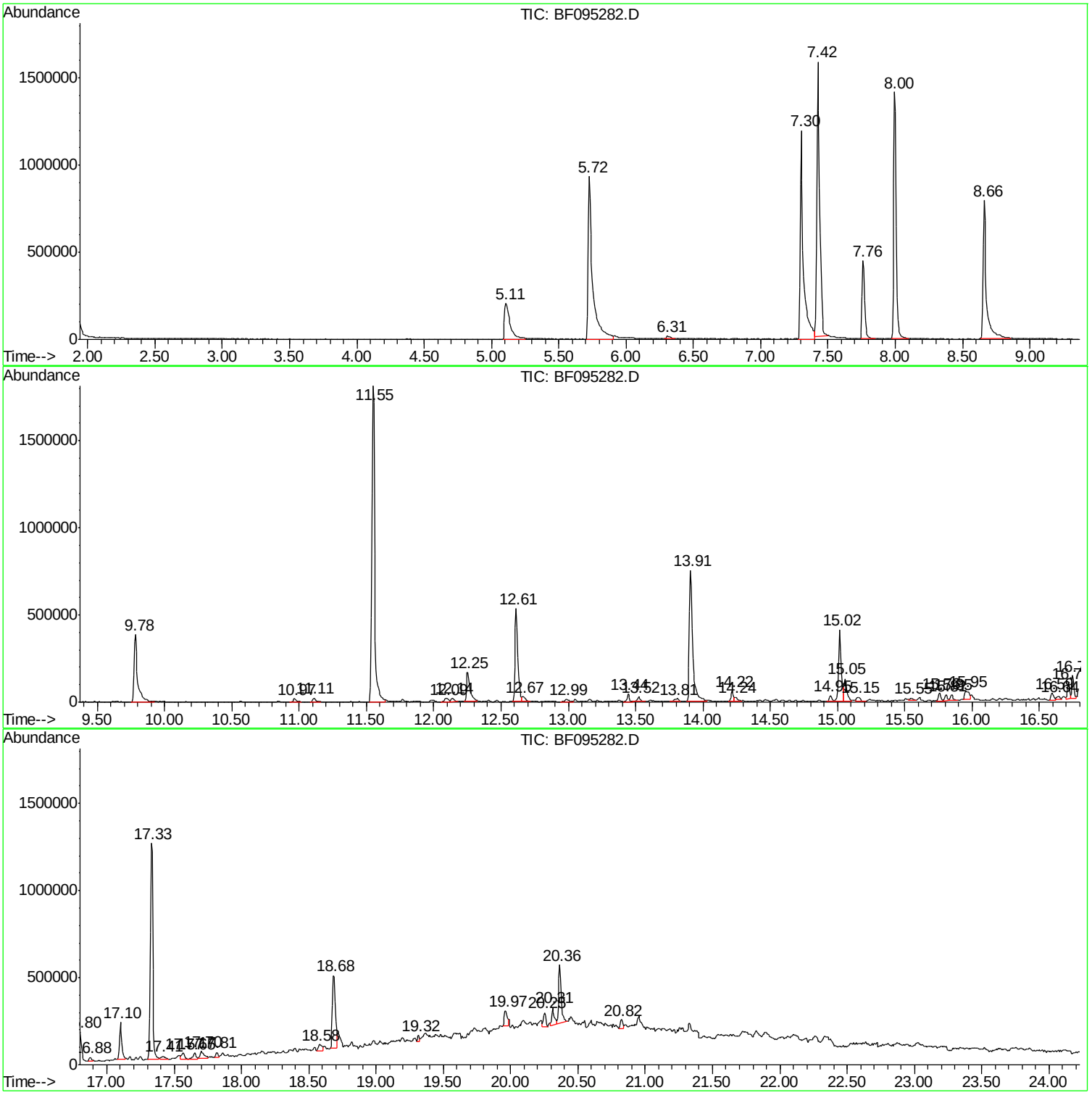
Sum of corrected areas: 22339843

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095282.D
Acq On : 20 May 2017 1:23
Operator : SJ/MA
Sample : I3202-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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\BF051917\
Data File : BF095282.D
Acq On : 20 May 2017 1:23
Operator : SJ/MA
Sample : I3202-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

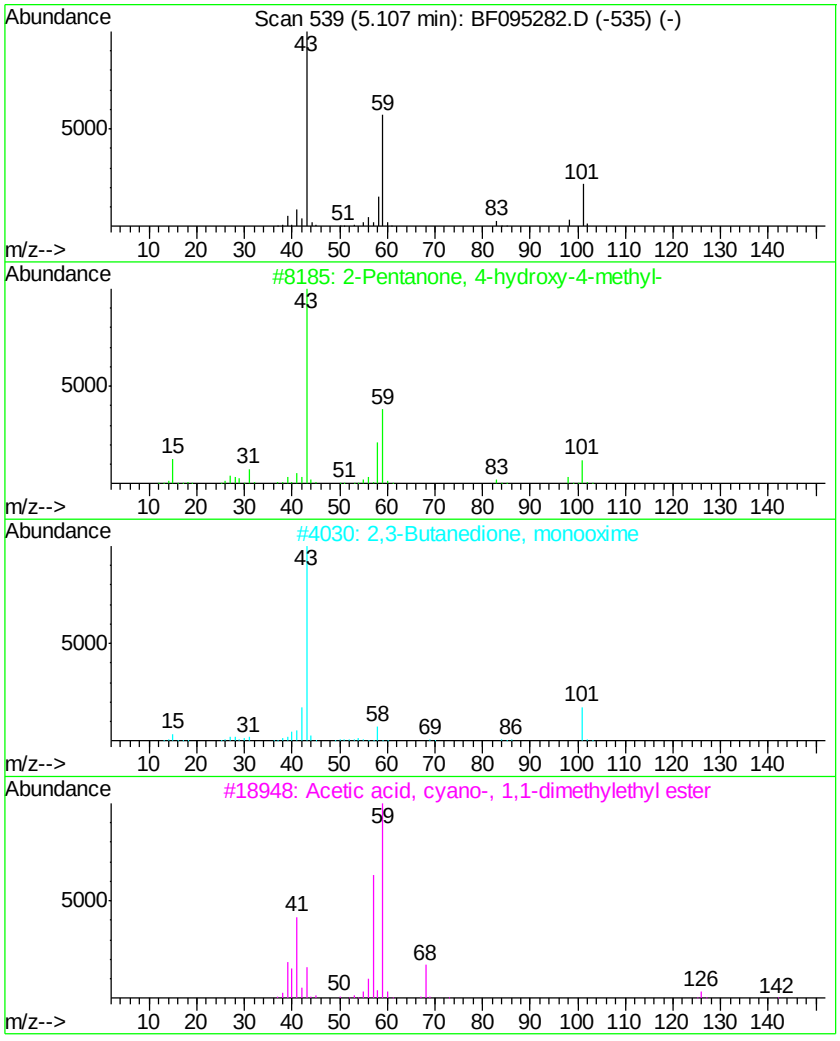
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

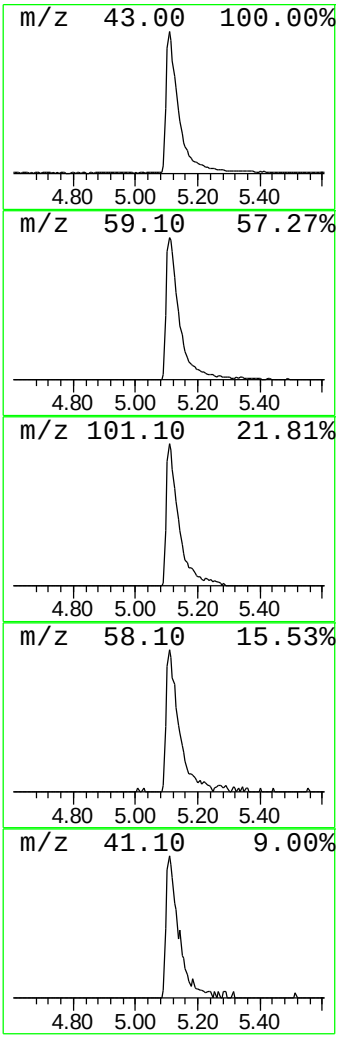
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	20.38 ng	568551	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095282.D
Acq On : 20 May 2017 1:23
Operator : SJ/MA
Sample : I3202-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

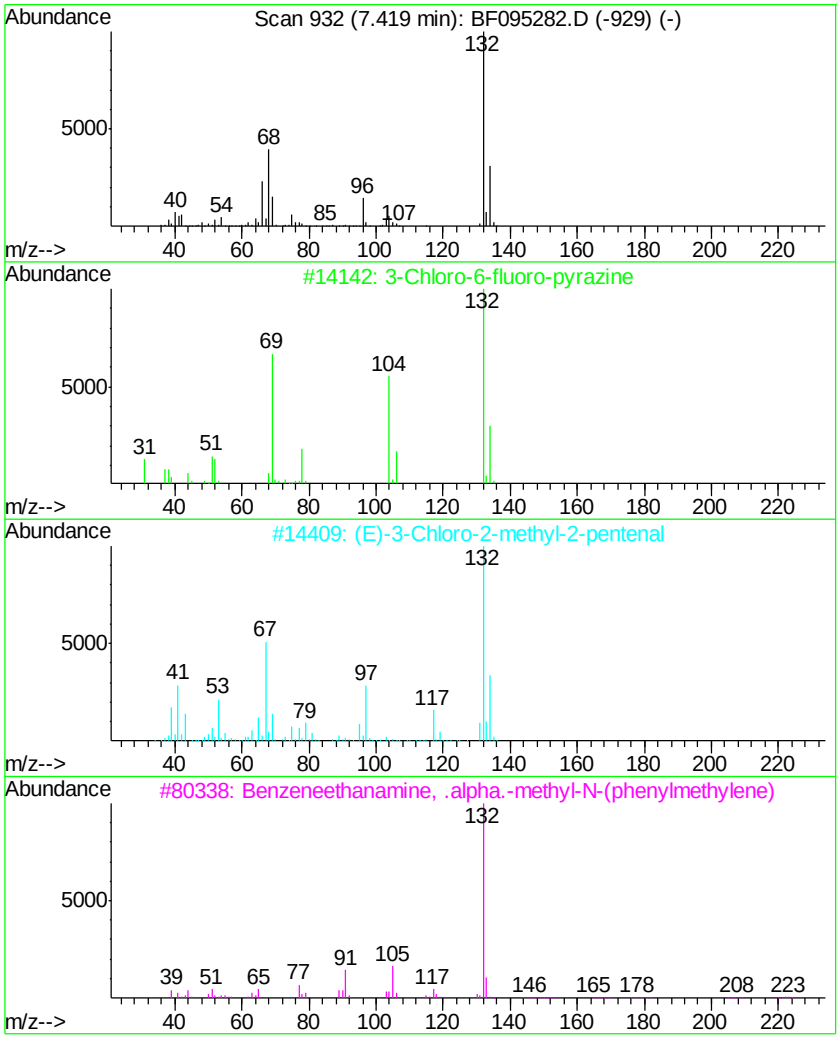
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

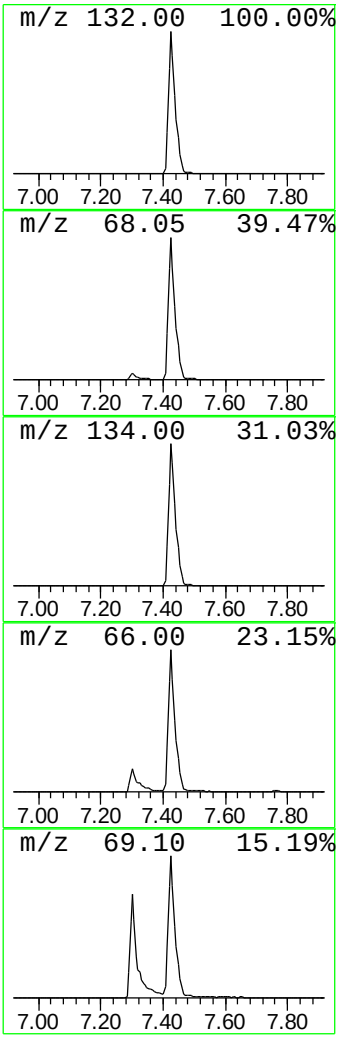
****

Peak Number 2 unknown7.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	87.26 ng	2434500	1,4-Dichlorobenzene-d4	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	Benzeneethanamine, .alpha.-methy...	223	C16H17N	002980-02-1	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095282.D
Acq On : 20 May 2017 1:23
Operator : SJ/MA
Sample : I3202-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

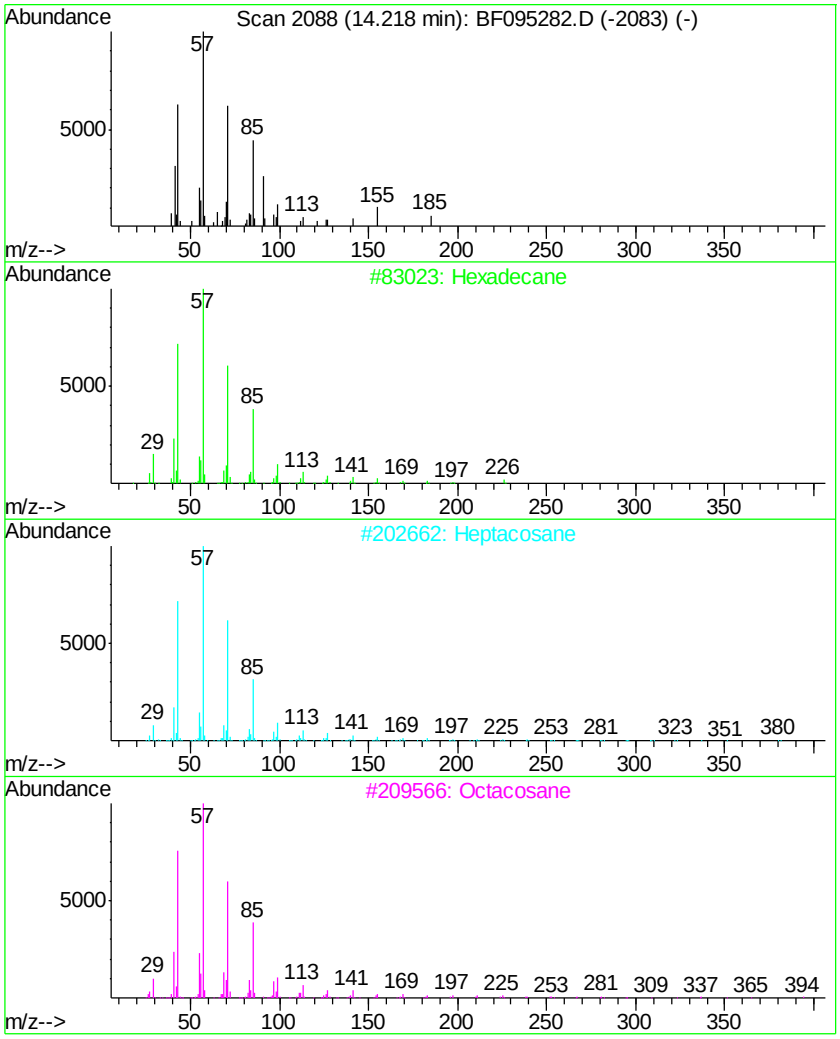
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

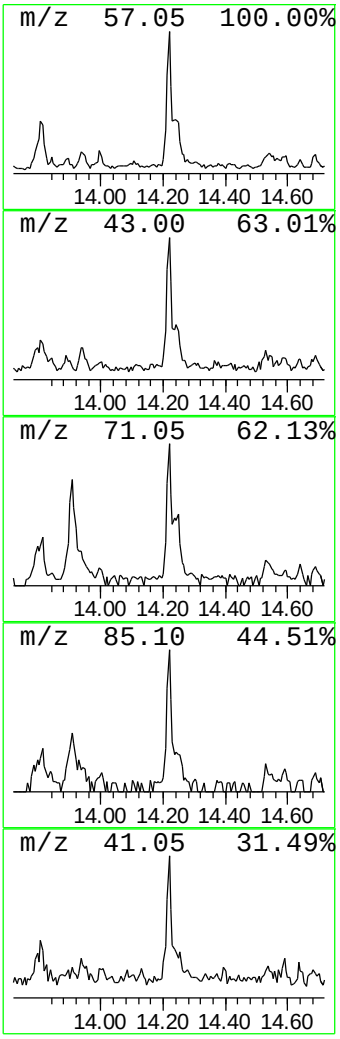
****

Peak Number 4 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.22	2.08 ng	64436	Phenanthrene-d10	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Heptacosane	380	C27H56	000593-49-7	86
3	Octacosane	394	C28H58	000630-02-4	83
4	Tetratetracontane	619	C44H90	007098-22-8	80
5	10-Methylnonadecane	282	C20H42	056862-62-5	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095282.D
Acq On : 20 May 2017 1:23
Operator : SJ/MA
Sample : I3202-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

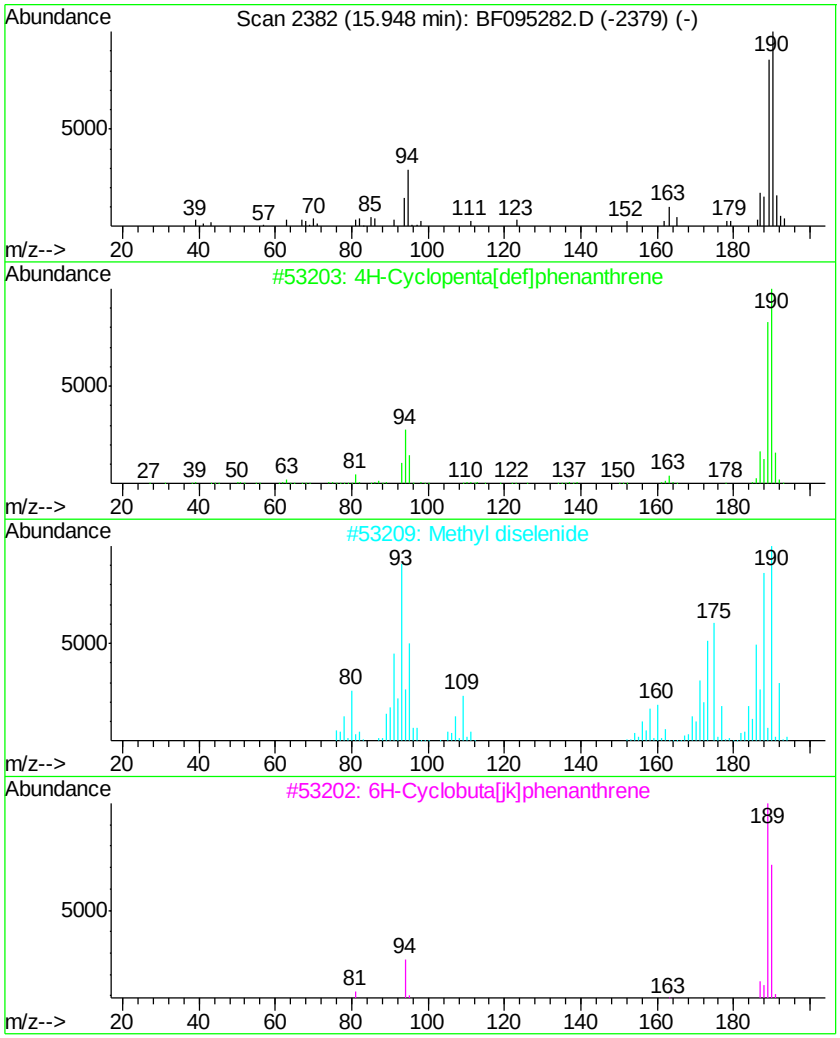
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

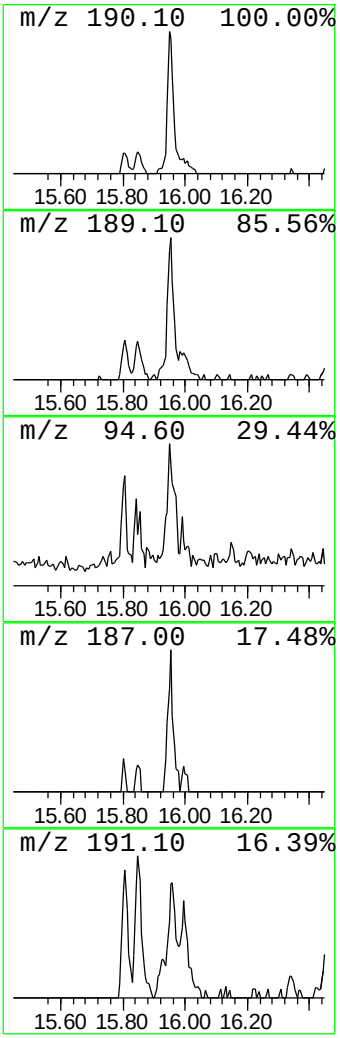
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	3.78 ng	116806	Phenanthrene-d10	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	72
2	Methyl diselenide	190	C2H6Se2	007101-31-7	60
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
4	1-Aminocyclopentanecarboxylic ac...	431	C23H42ClNO4	1000329-17-4	22
5	Carbonic acid, butyl 2-formyl-4,...	290	C12H12Cl2O4	1000331-42-2	17





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095282.D
Acq On : 20 May 2017 1:23
Operator : SJ/MA
Sample : I3202-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

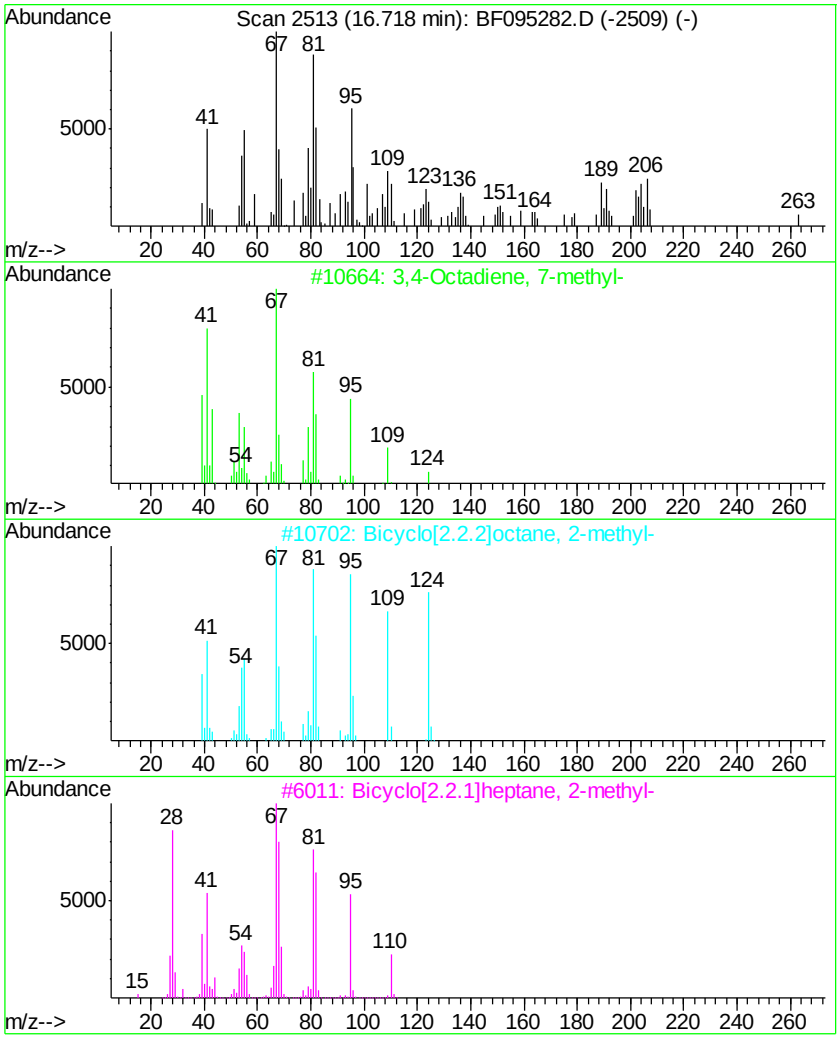
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

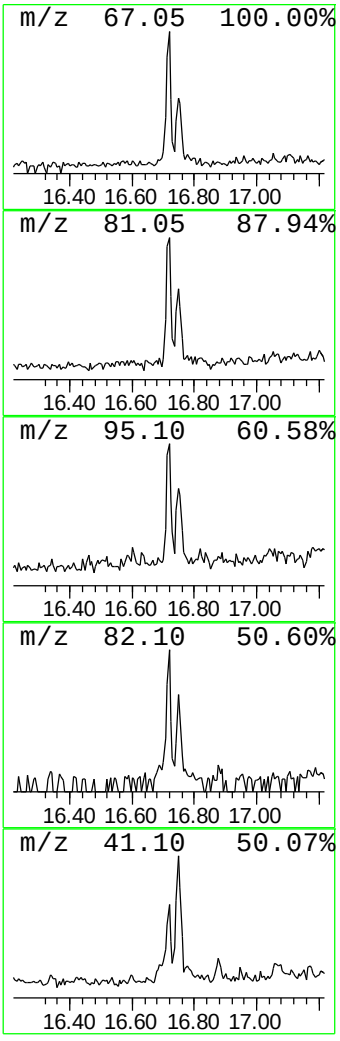
****

Peak Number 6 3,4-Octadiene, 7-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	3.29 ng	101579	Phenanthrene-d10	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	64
2	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	58
3	Bicyclo[2.2.1]heptane, 2-methyl-	110	C8H14	015185-11-2	52
4	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	49
5	Cyclobuta[1,2:3,4]dicyclooctene,...	220	C16H28	017385-55-6	46





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095282.D
Acq On : 20 May 2017 1:23
Operator : SJ/MA
Sample : I3202-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

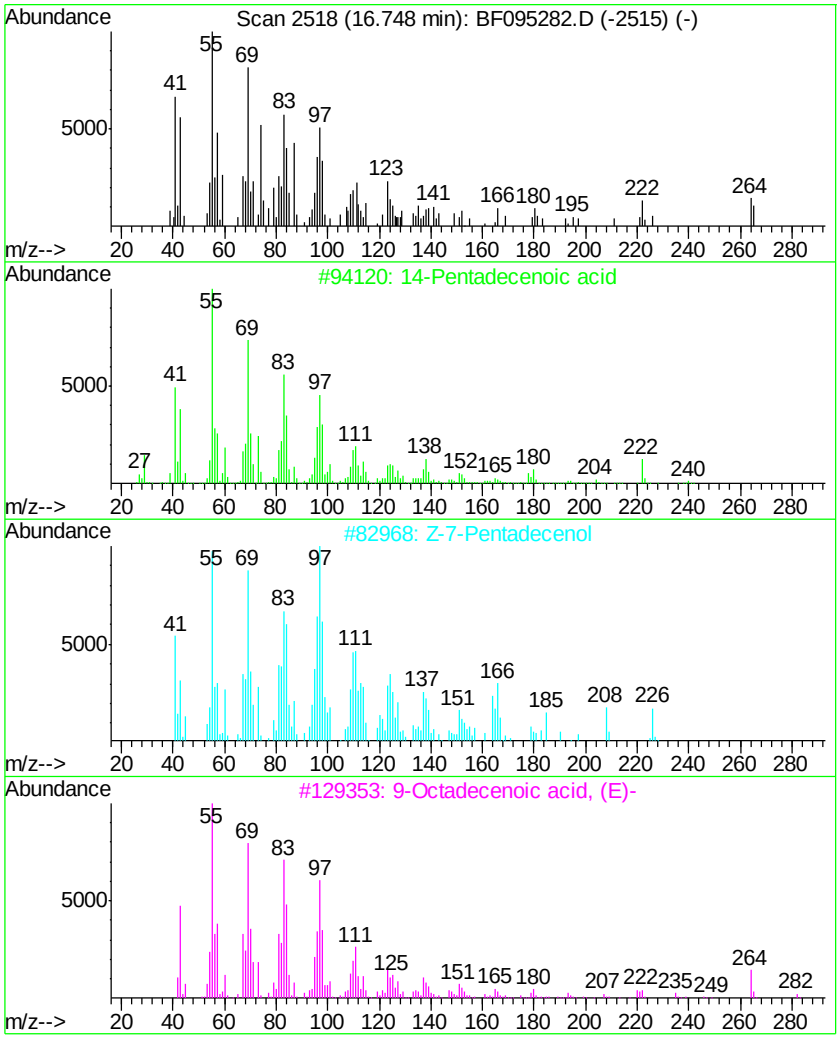
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

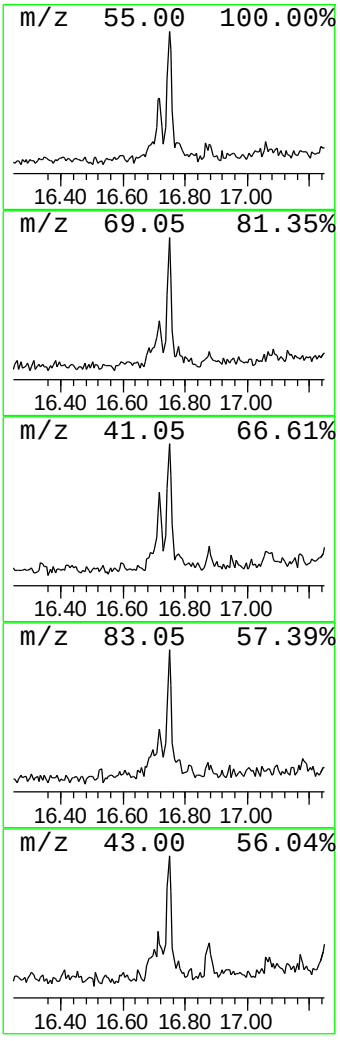
****

Peak Number 7 14-Pentadecenoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.75	4.76 ng	147067	Phenanthrene-d10	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	14-Pentadecenoic acid	240	C15H28O2	017351-34-7	76
2	Z-7-Pentadecenol	226	C15H30O	1000130-76-6	70
3	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	68
4	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	64
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	58





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095282.D
Acq On : 20 May 2017 1:23
Operator : SJ/MA
Sample : I3202-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

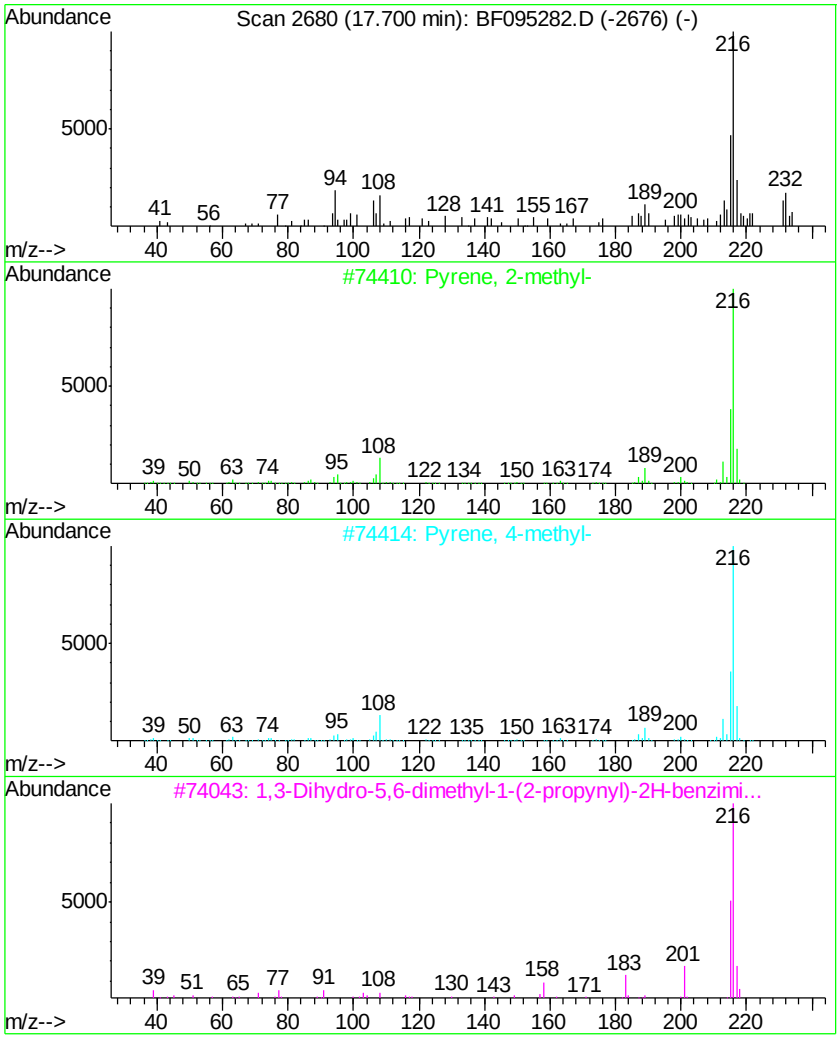
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

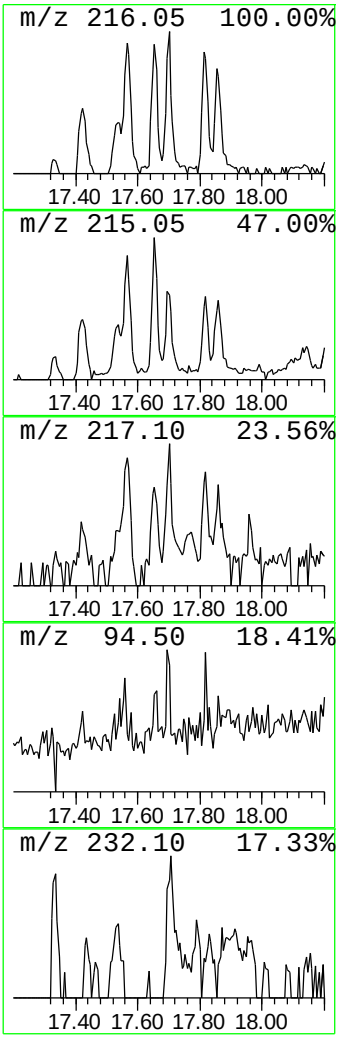
****

Peak Number 8 Pyrene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.70	2.53 ng	79887	Chrysene-d12	18.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	76
2	Pyrene, 4-methyl-	216	C17H12	003353-12-6	76
3	1,3-Dihydro-5,6-dimethyl-1-(2-pr...	216	C12H12N2S	080276-22-8	59
4	1,2-Difluorostilbene	216	C14H10F2	000643-76-5	59
5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	58





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095282.D
Acq On : 20 May 2017 1:23
Operator : SJ/MA
Sample : I3202-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

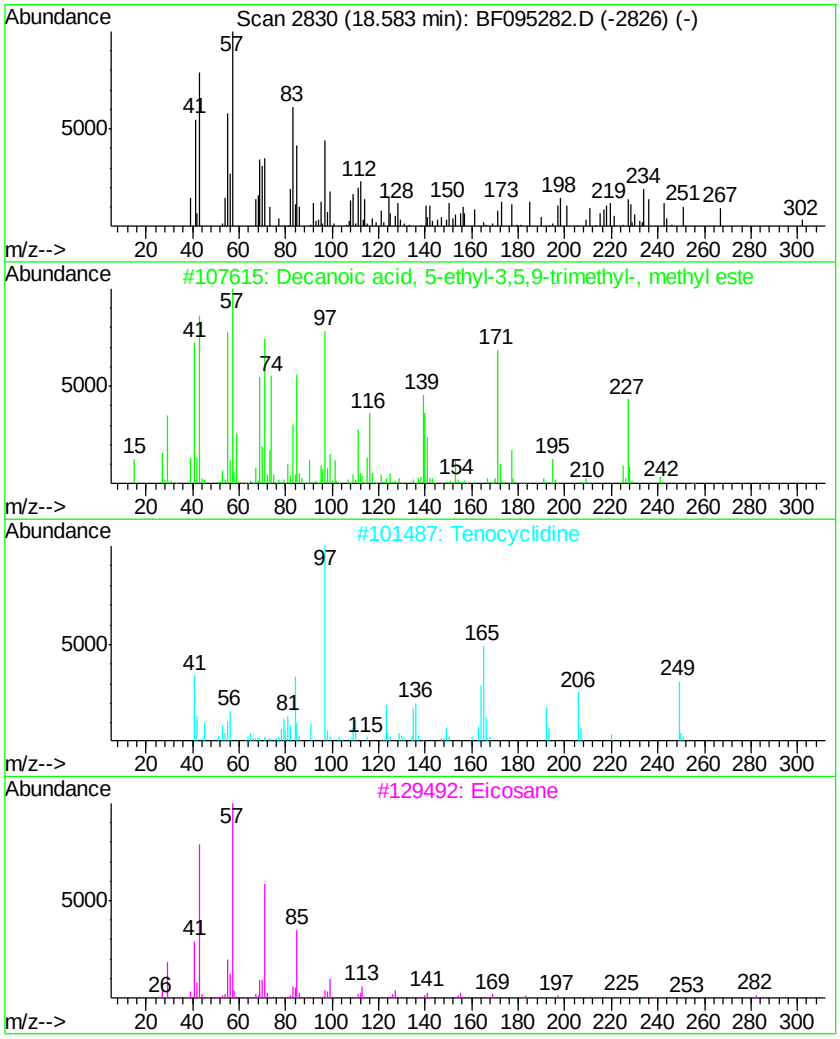
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

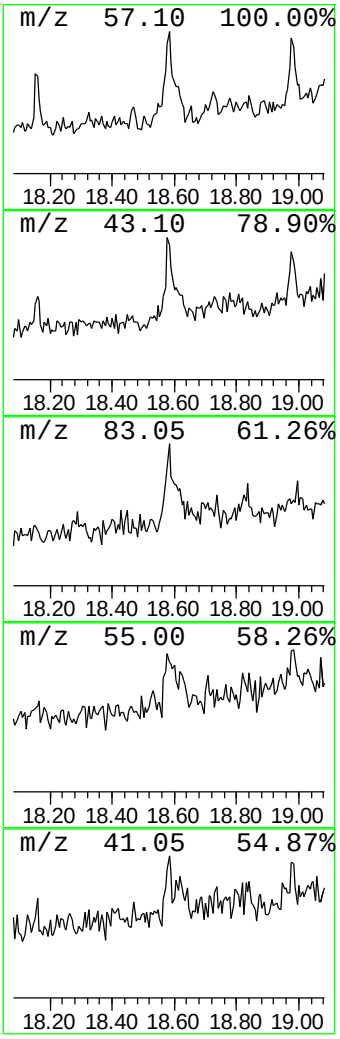
****

Peak Number 9 unknown18.58 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	2.31 ng	72905	Chrysene-d12	18.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanoic acid, 5-ethyl-3,5,9-tri...	256	C16H32O2	056247-63-3	35
2	Tenocyclidine	249	C15H23NS	021500-98-1	25
3	Eicosane	282	C20H42	000112-95-8	18
4	Penta-2,4-dien-1-one, 5,5-dichlo...	230	C10H8Cl2O2	177754-30-2	15
5	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	14





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095282.D
Acq On : 20 May 2017 1:23
Operator : SJ/MA
Sample : I3202-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

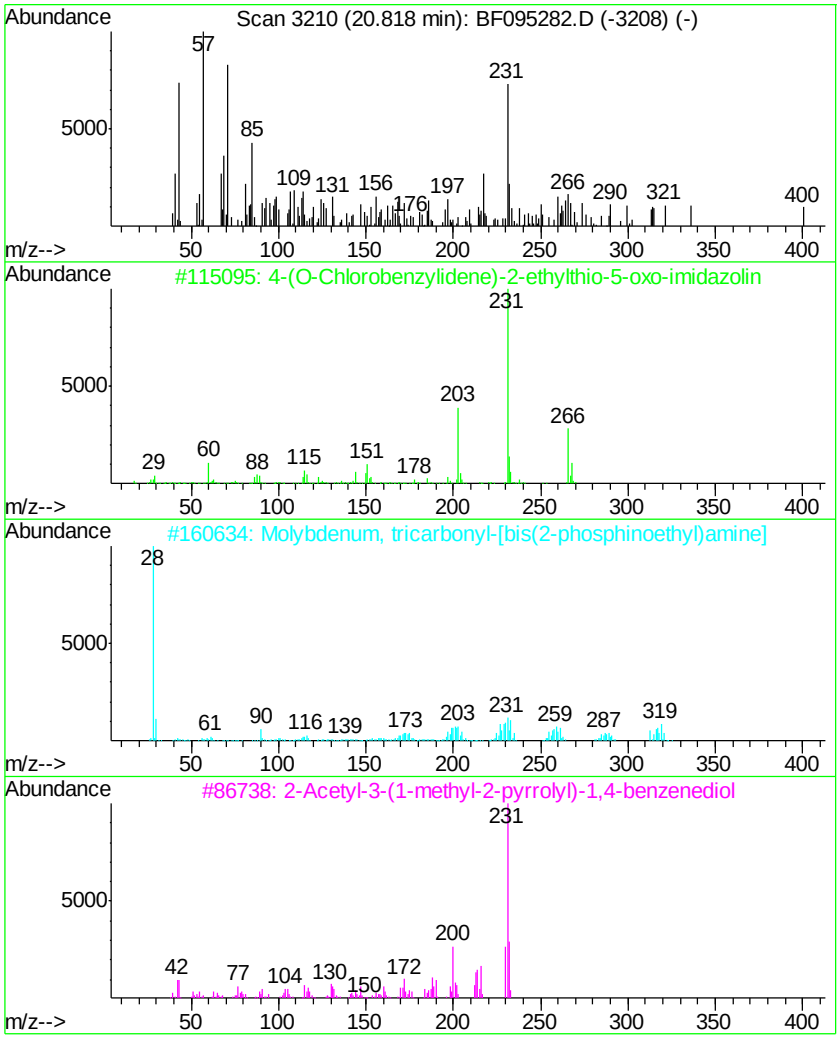
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

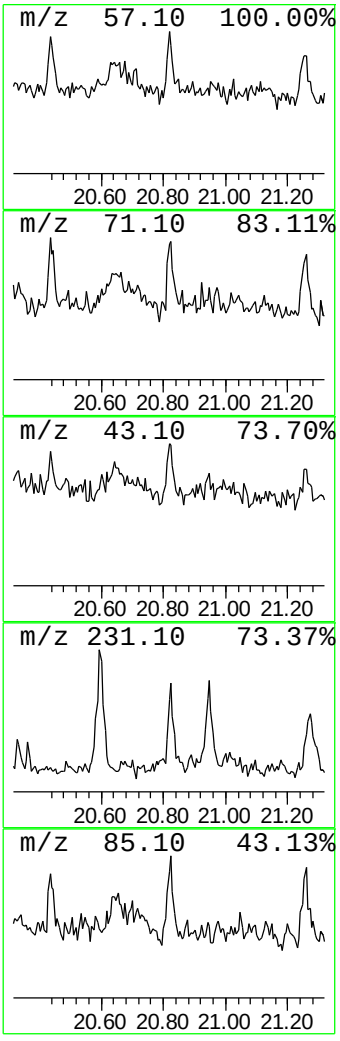
****

Peak Number 11 unknown20.82 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.82	2.71 ng	61800	Perylene-d12	20.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(O-Chlorobenzylidene)-2-ethylt...	266	C12H11ClN2OS	033449-97-7	25
2	Molybdenum, tricarbonyl-[bis(2-p...	319	C7H13MoNO3P2	1000162-16-7	22
3	2-Acetyl-3-(1-methyl-2-pyrrolyl)...	231	C13H13NO3	1000326-75-5	22
4	Pentadecane, 8,8-diheptyl-	408	C29H60	055268-72-9	22
5	2-Mercaptophenothiazine	231	C12H9NS2	099970-41-9	20





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095282.D
Acq On : 20 May 2017 1:23
Operator : SJ/MA
Sample : I3202-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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...	5.11	20.4	ng	568551	1	7.76	558015	20.0
unknown7.42	7.42	87.3	ng	2434500	1	7.76	558015	20.0
Hexadecane	14.22	2.1	ng	64436	4	15.02	618431	20.0
4H-Cyclopenta[def...	15.95	3.8	ng	116806	4	15.02	618431	20.0
3,4-Octadiene, 7-...	16.72	3.3	ng	101579	4	15.02	618431	20.0
14-Pentadecenoic ...	16.75	4.8	ng	147067	4	15.02	618431	20.0
Pyrene, 2-methyl-	17.70	2.5	ng	79887	5	18.69	631427	20.0
unknown18.58	18.58	2.3	ng	72905	5	18.69	631427	20.0
unknown20.82	20.82	2.7	ng	61800	6	20.36	456168	20.0