LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095575.D
Acq On : 31 May 2017 21:12
Operator : SJ/MA
Sample : I3341-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM11-COMP-0-6

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	4.813	502	506	528	rBV	80835	227286	8.44%	0.836%
2	5.472	614	618	648	rBV	1177403	2386262	88.66%	8.781%
3	7.107	891	896	909	rBV	1339989	2203212	81.86%	8.107%
4	7.213	909	914	932	rVB	1762621	2691442	100.00%	9.904%
5	7.554	967	972	985	rBV	412732	545515	20.27%	2.007%
6	7.789	1007	1012	1030	rBV	1376142	1808915	67.21%	6.656%
7	8.466	1122	1127	1151	rBV	953186	1466796	54.50%	5.398%
8	9.583	1312	1317	1329	rBV	580859	827568	30.75%	3.045%
9	11.360	1613	1619	1633	rBV	2044084	2495424	92.72%	9.183%
10	12.048	1731	1736	1749	rBV	483112	607896	22.59%	2.237%
11	12.407	1792	1797	1804	rBV2	721009	916210	34.04%	3.371%
12	12.460	1804	1806	1811	rVB	42669	52061	1.93%	0.192%
13	12.765	1855	1858	1865	rBV2	15276	28221	1.05%	0.104%
14	13.254	1937	1941	1946	rVB	38135	43688	1.62%	0.161%
15	13.312	1946	1951	1959	rBV	43474	62501	2.32%	0.230%
16	13.707	2013	2018	2032	rBV	904233	1306927	48.56%	4.809%
17	14.024	2067	2072	2080	rBV	43259	68898	2.56%	0.254%
18	14.759	2192	2197	2200	rBV	24480	29355	1.09%	0.108%
19	14.806	2200	2205	2209	rVV2	594355	766969	28.50%	2.822%
20	14.848	2209	2212	2218	rVV	395866	491563	18.26%	1.809%
21	14.942	2221	2228	2238	rVV	95186	150194	5.58%	0.553%
22	15.248	2276	2280	2287	rBV	21038	32851	1.22%	0.121%
23	15.318	2287	2292	2301	rVV4	57966	102537	3.81%	0.377%
24	15.606	2338	2341	2345	rVB	54974	52730	1.96%	0.194%
25	15.648	2345	2348	2351	rBV	66526	71271	2.65%	0.262%
26	15.683	2351	2354	2358	rBV2	37188	48950	1.82%	0.180%
27	15.736	2358	2363	2365	rBV2	67907	96912	3.60%	0.357%
28	15.801	2370	2374	2383	rVB	201063	272799	10.14%	1.004%
29	16.053	2414	2417	2426	rVB	38716	45979	1.71%	0.169%
30	16.406	2474	2477	2481	rBV	30777	37601	1.40%	0.138%
31	16.524	2493	2497	2502	rVB5	17137	30046	1.12%	0.111%
32	16.606	2507	2511	2517	rBV	468845	538083	19.99%	1.980%
33	16.695	2522	2526	2531	rVB3	45711	49246	1.83%	0.181%
34	16.806	2541	2545	2550	rVB3	23336	35311	1.31%	0.130%

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Misc :
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Instrument : BNA_F
ClientSampleId : NM11-COMP-0-6

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

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Peak separation: 5

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

35	16.912	2556	2563	2569	rBV	456096	552113	20.51%	2.032%
36	17.106	2593	2596	2600	rBV2	27845	27980	1.04%	0.103%
37	17.153	2600	2604	2610	rVV	1371593	1592328	59.16%	5.859%
38	17.236	2612	2618	2625	rVB4	24066	50340	1.87%	0.185%
39	17.347	2633	2637	2640	rBV4	18655	36585	1.36%	0.135%
40	17.383	2640	2643	2648	rVB	59864	69352	2.58%	0.255%
41	17.465	2654	2657	2662	rVB	36468	44706	1.66%	0.165%
42	17.512	2662	2665	2670	rBV4	57411	91193	3.39%	0.336%
43	17.630	2682	2685	2689	rVB	22761	27943	1.04%	0.103%
44	17.836	2713	2720	2721	rBV7	13847	28667	1.07%	0.105%
45	17.853	2721	2723	2728	rVB	57057	60264	2.24%	0.222%
46	18.071	2757	2760	2764	rVB	23770	30255	1.12%	0.111%
47	18.212	2781	2784	2787	rVB2	42115	43931	1.63%	0.162%
48	18.247	2787	2790	2793	rBV	23591	27018	1.00%	0.099%
49	18.283	2793	2796	2801	rVV2	25879	29381	1.09%	0.108%
50	18.342	2803	2806	2812	rVV2	28120	37977	1.41%	0.140%
51	18.400	2812	2816	2825	rBV3	96472	165279	6.14%	0.608%
52	18.500	2827	2833	2837	rVV2	598014	829243	30.81%	3.051%
53	18.541	2837	2840	2851	rVB3	161780	285593	10.61%	1.051%
54	18.636	2851	2856	2859	rBV2	39596	52219	1.94%	0.192%
55	19.018	2914	2921	2924	rVB	49901	73649	2.74%	0.271%
56	19.053	2924	2927	2931	rVB2	24408	29695	1.10%	0.109%
57	19.200	2949	2952	2960	rVV5	43194	75713	2.81%	0.279%
58	19.406	2981	2987	2990	rBV8	15060	27997	1.04%	0.103%
59	19.447	2990	2994	3000	rVV9	16990	35264	1.31%	0.130%
60	19.636	3020	3026	3029	rBV6	32175	48450	1.80%	0.178%
61	19.724	3038	3041	3045	rBV4	52496	66700	2.48%	0.245%
62	19.777	3045	3050	3053	rBV	196161	269076	10.00%	0.990%
63	19.888	3066	3069	3072	rBV	38355	38490	1.43%	0.142%
64	19.924	3072	3075	3077	rBV	61022	77422	2.88%	0.285%
65	20.065	3095	3099	3103	rBV	117752	133161	4.95%	0.490%
66	20.124	3106	3109	3114	rBV	162195	168162	6.25%	0.619%
67	20.177	3114	3118	3122	rBV	431712	492273	18.29%	1.811%
68	20.424	3157	3160	3165	rBV6	33002	34593	1.29%	0.127%
69	20.618	3188	3193	3197	rBV	188287	286866	10.66%	1.056%
70	20.665	3198	3201	3209	rVB5	67737	128491	4.77%	0.473%
71	21.382	3319	3323	3324	rBV3	20335	26927	1.00%	0.099%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	21.430	3327	3331	3334	rVV	77802	128492	4.77%	0.473%
73	21.477	3335	3339	3347	rVB5	125433	230387	8.56%	0.848%
74	21.794	3388	3393	3397	rBV	60890	129968	4.83%	0.478%

Sum of corrected areas: 27175362

LSC Report - Integrated Chromatogram

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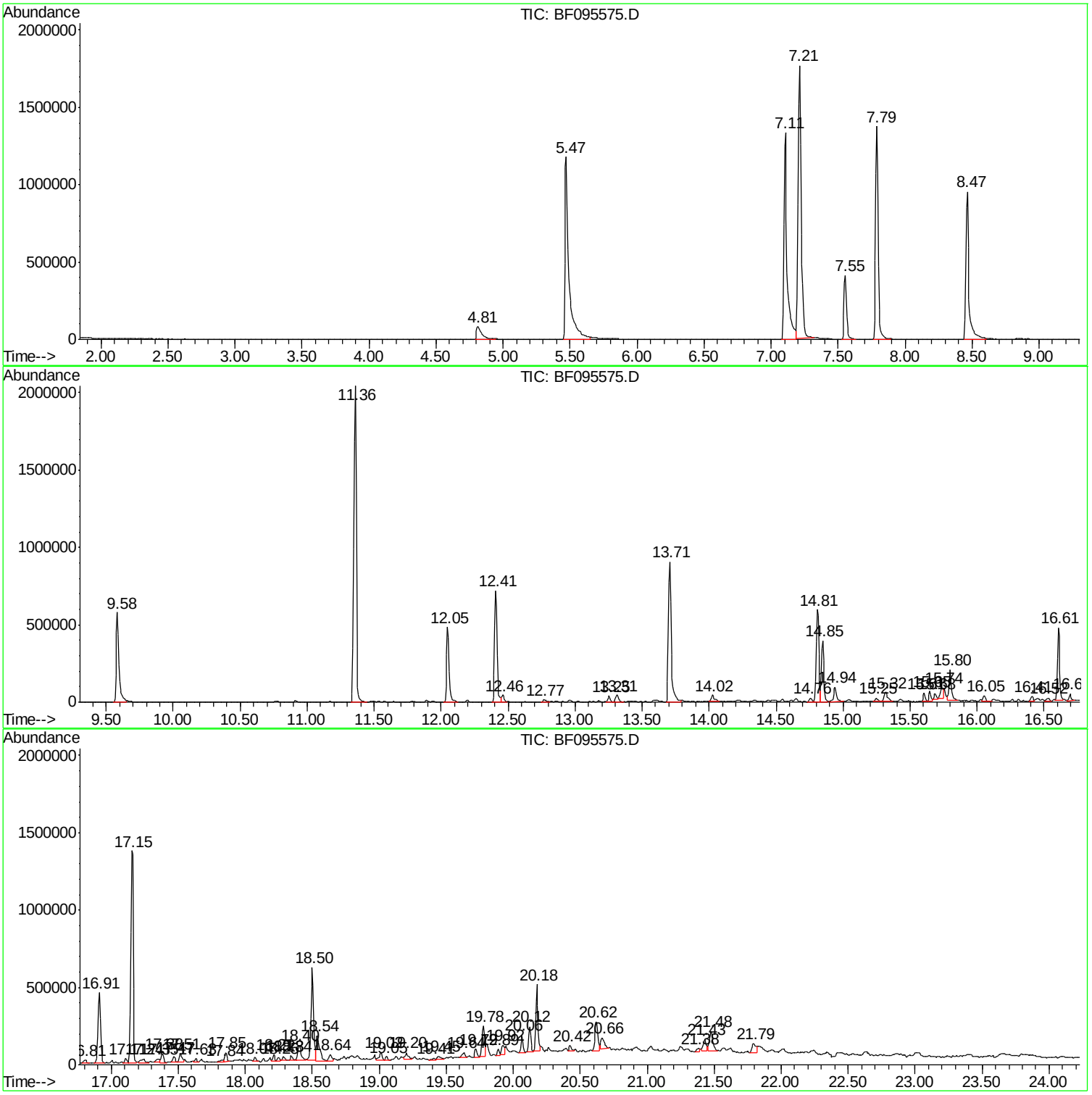
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM11-COMP-0-6

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\BF053117\
Data File : BF095575.D
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Operator : SJ/MA
Sample : I3341-01
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Instrument : BNA_F
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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

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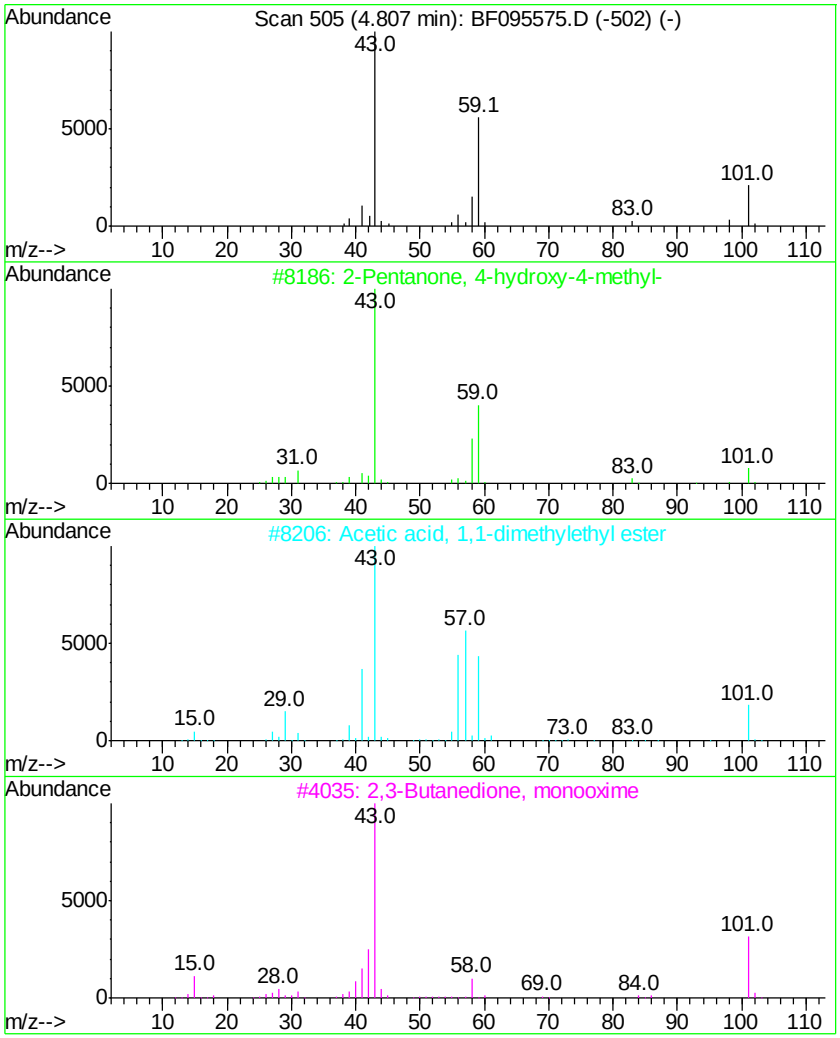
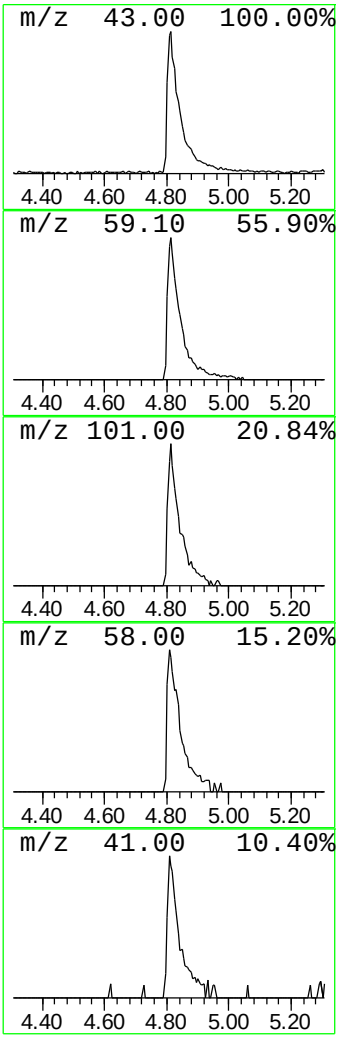
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	8.33 ng	227286	1,4-Dichlorobenzene-d4	7.55

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	38
4	3-Hexanol	102	C6H14O	000623-37-0	28
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25





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Instrument : BNA_F
ClientSampleId : NM11-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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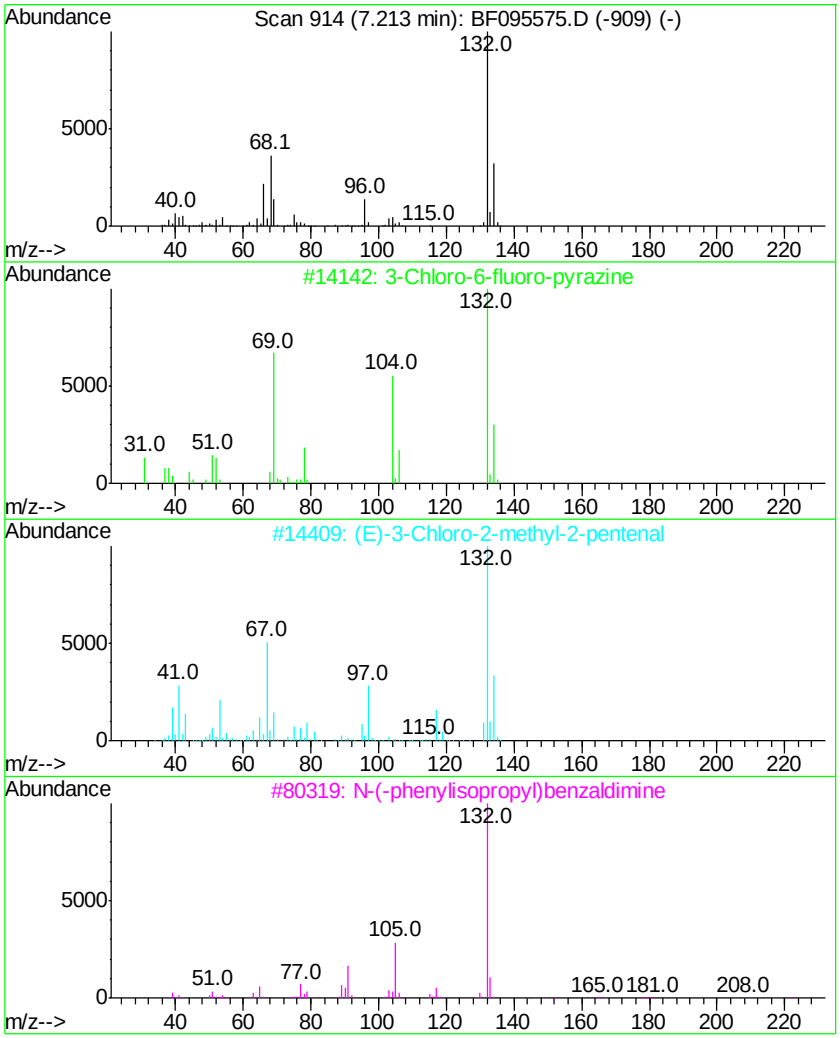
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

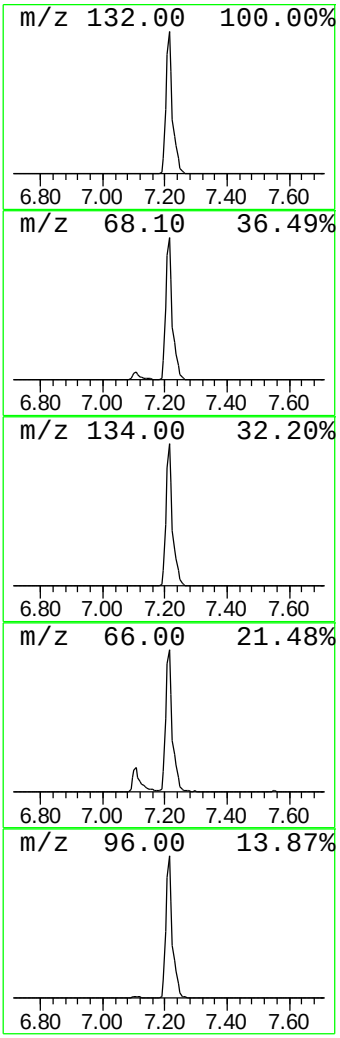
****

Peak Number 2 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	98.68 ng	2691440	1,4-Dichlorobenzene-d4	7.55

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	N-(-phenylisopropyl)benzaldimine	223	C16H17N	1000379-01-3	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	Benzeneethanamine, .alpha.-methy...	223	C16H17N	002980-02-1	12





Library Search Compound Report

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Sample : I3341-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM11-COMP-0-6

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

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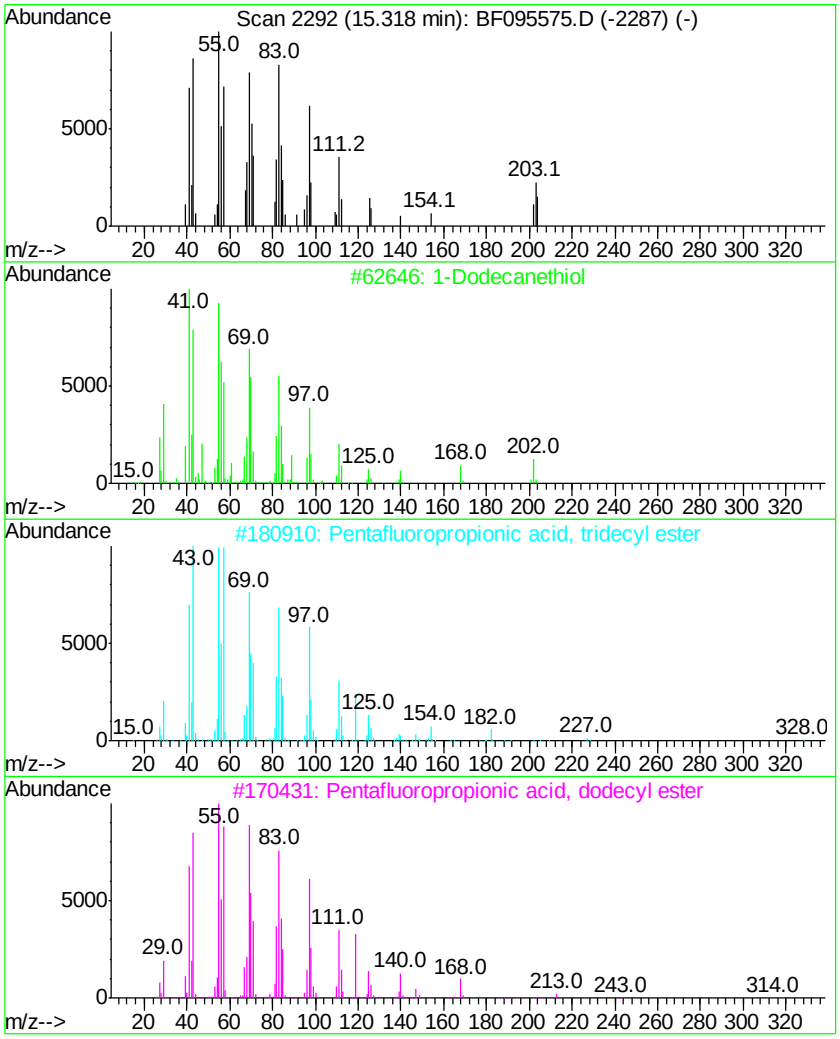
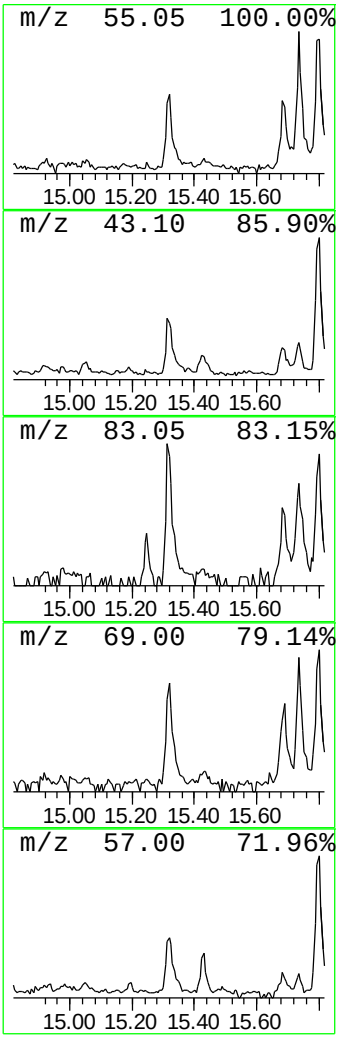
Peak Number 4 1-Dodecanethiol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	2.67 ng	102537	Phenanthrene-d10	14.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanethiol	202	C12H26S	000112-55-0	96
2	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	94
3	Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	94
4	Pentafluoropropionic acid, undec...	318	C14H23F5O2	959014-11-0	94
5	Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	91





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Instrument : BNA_F
ClientSampleId : NM11-COMP-0-6

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

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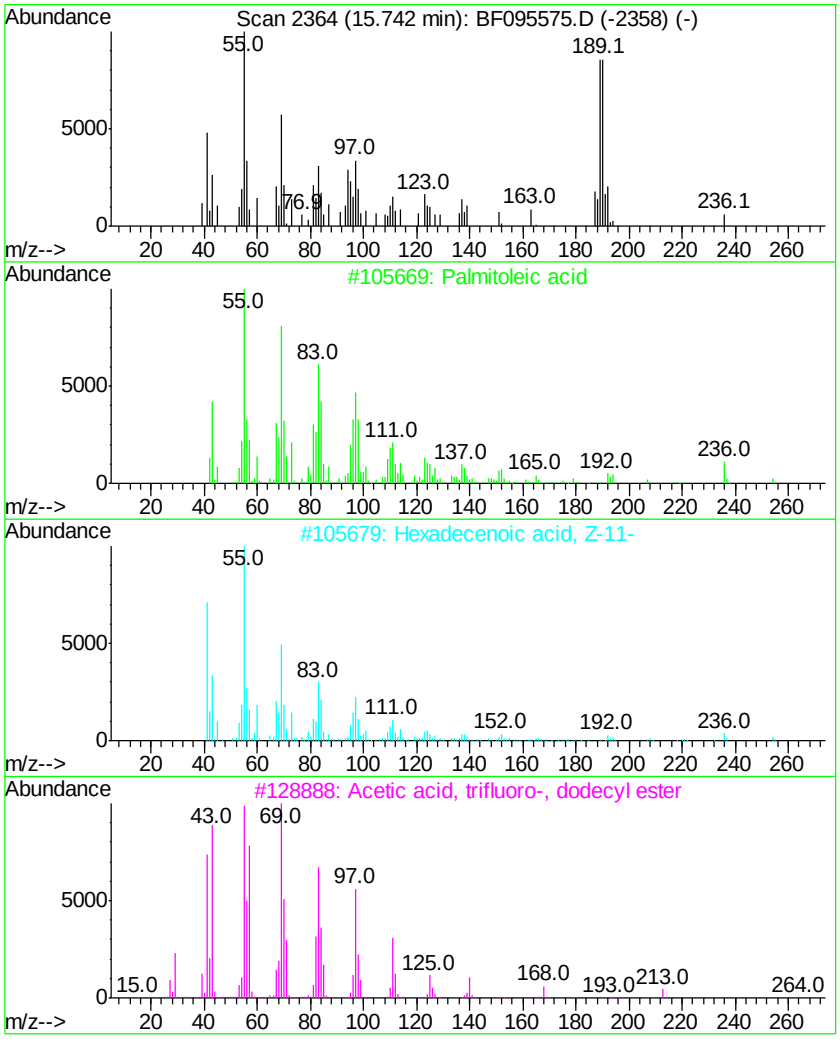
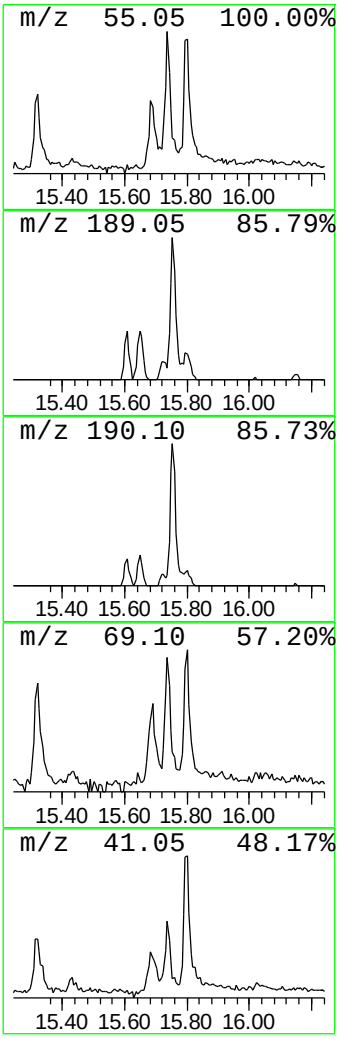
Peak Number 5 unknown15.74 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	2.53 ng	96912	Phenanthrene-d10	14.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleic acid	254	C16H30O2	000373-49-9	43
2	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	35
3	Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	27
4	7,11-Hexadecadienal	236	C16H28O	1000130-85-7	22
5	Z-7-Tetradecenoic acid	226	C14H26O2	1000130-98-4	18





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TIC Library : C:\DATABASE\NIST11.L
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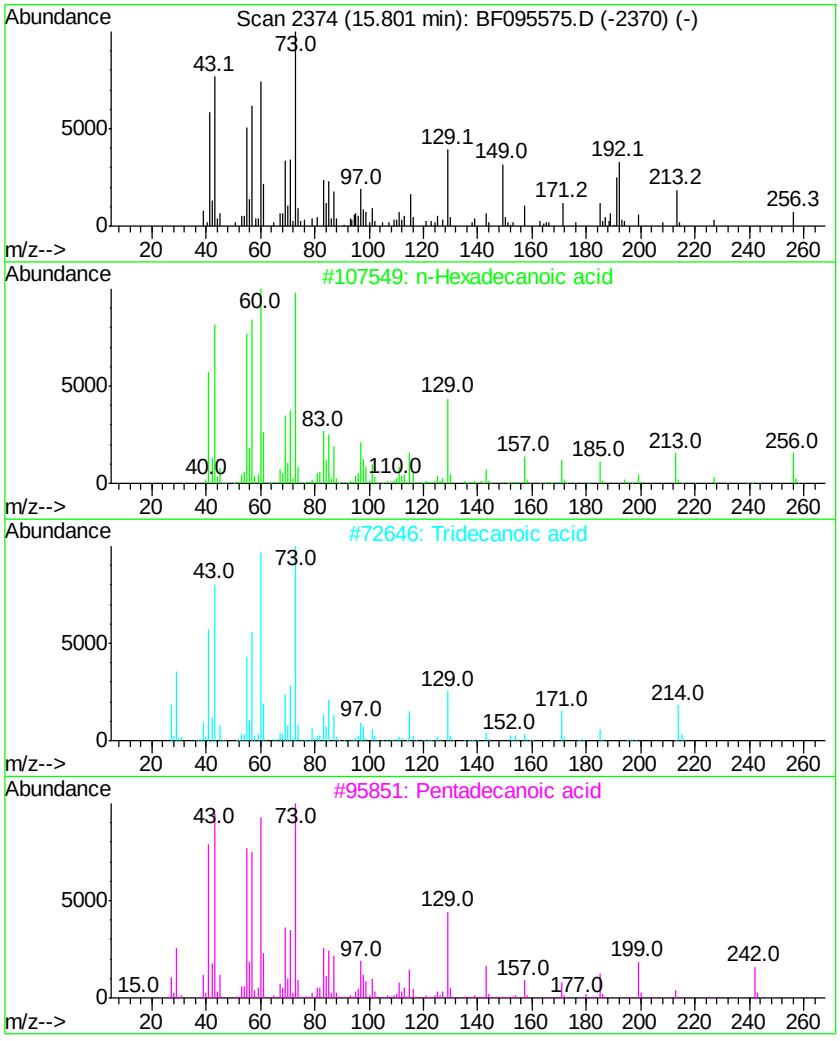
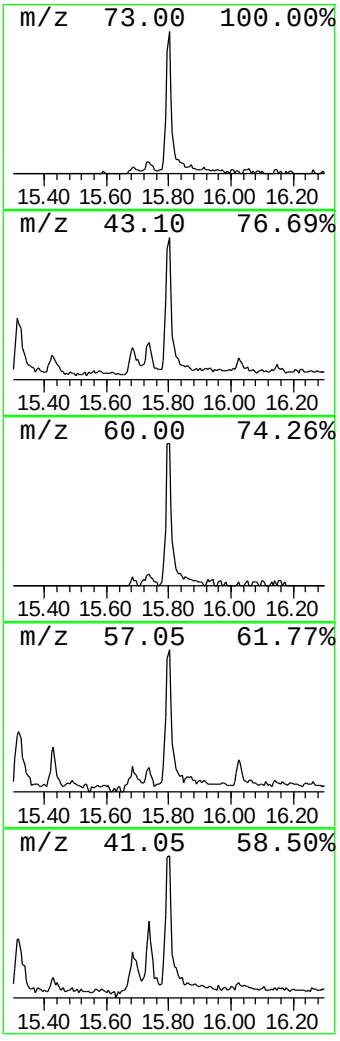
Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	7.11 ng	272799	Phenanthrene-d10	14.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	52





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Instrument : BNA_F
ClientSampleId : NM11-COMP-0-6

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

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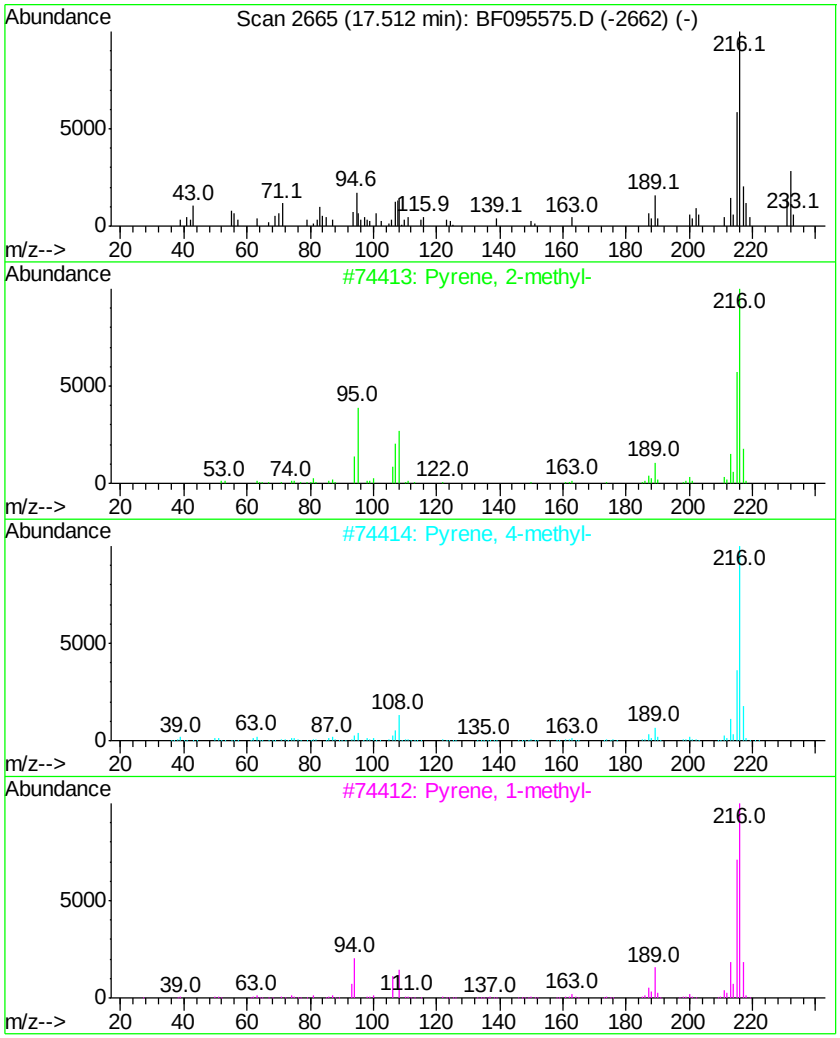
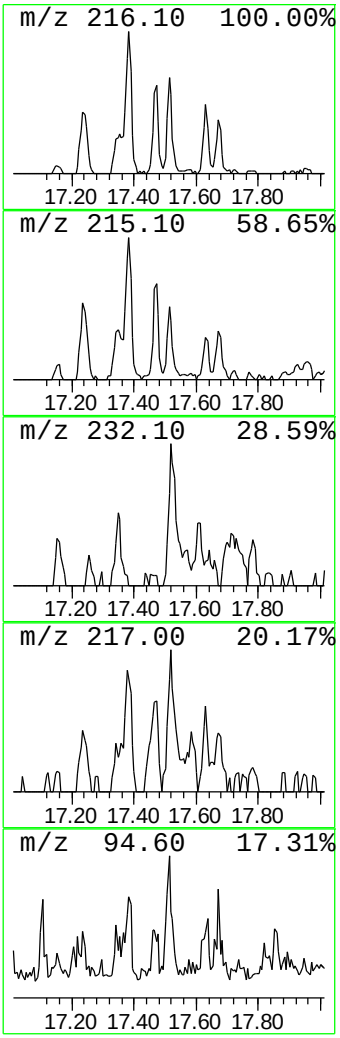
Peak Number 7 Pyrene, 2-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.51	2.20 ng	91193	Chrysene-d12	18.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	90
2	Pyrene, 4-methyl-	216	C17H12	003353-12-6	86
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	86
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	70
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	68





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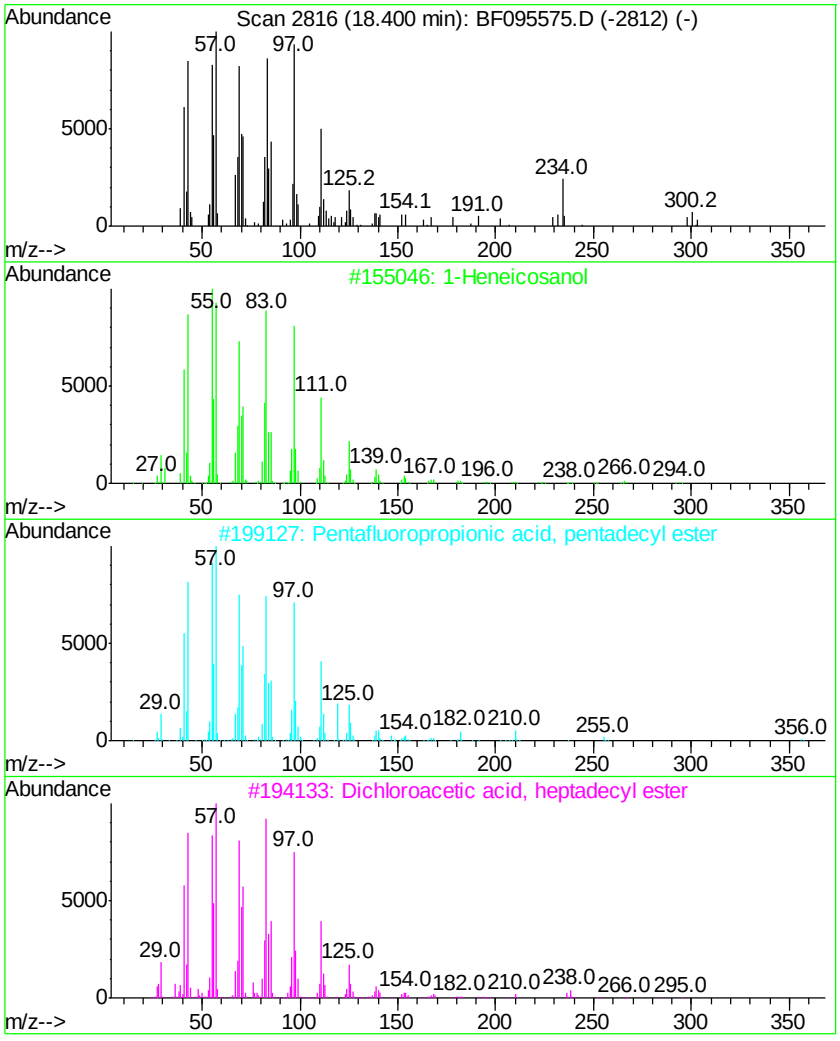
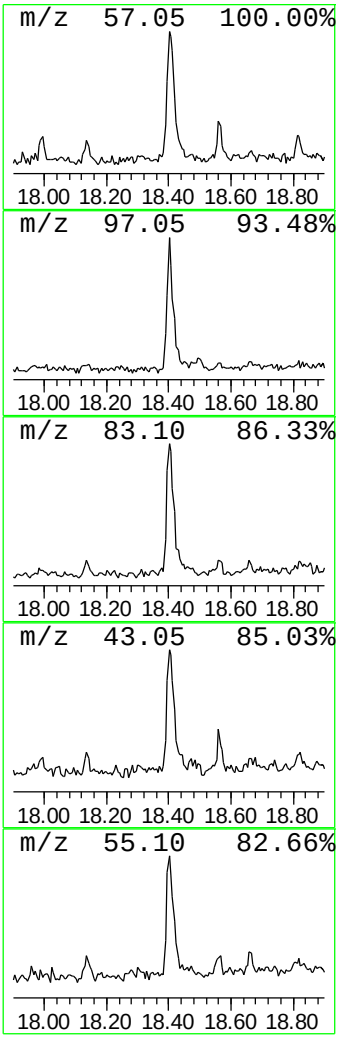
Peak Number 8 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	3.99 ng	165279	Chrysene-d12	18.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4	1-Nonadecene	266	C19H38	018435-45-5	90
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	87





Library Search Compound Report

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Data File : BF095575.D
Acq On : 31 May 2017 21:12
Operator : SJ/MA
Sample : I3341-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM11-COMP-0-6

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

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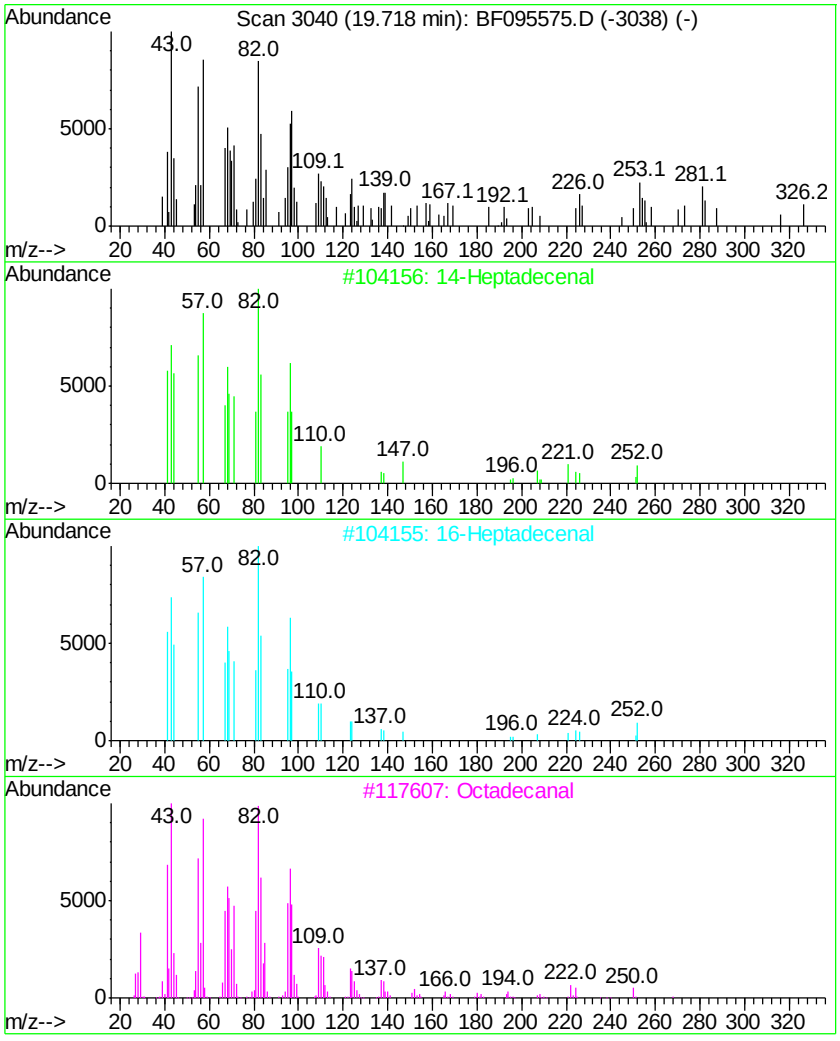
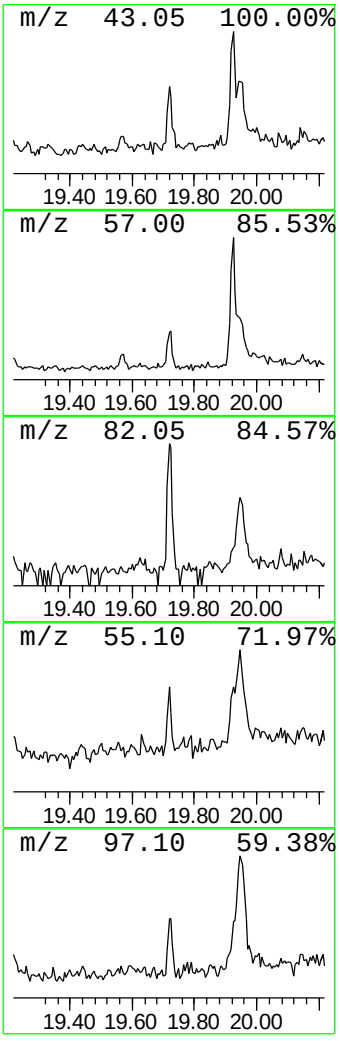
Peak Number 9 14-Heptadecenal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.72	2.71 ng	66700	Perylene-d12	20.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	14-Heptadecenal	252	C17H32O	1000144-58-0	55
2	16-Heptadecenal	252	C17H32O	1000144-57-9	55
3	Octadecanal	268	C18H36O	000638-66-4	53
4	E-8-Hexadecen-1-ol acetate	282	C18H34O2	1000131-01-1	49
5	1,13-Tridecanediol, diacetate	300	C17H32O4	042236-70-4	46





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Sample : I3341-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM11-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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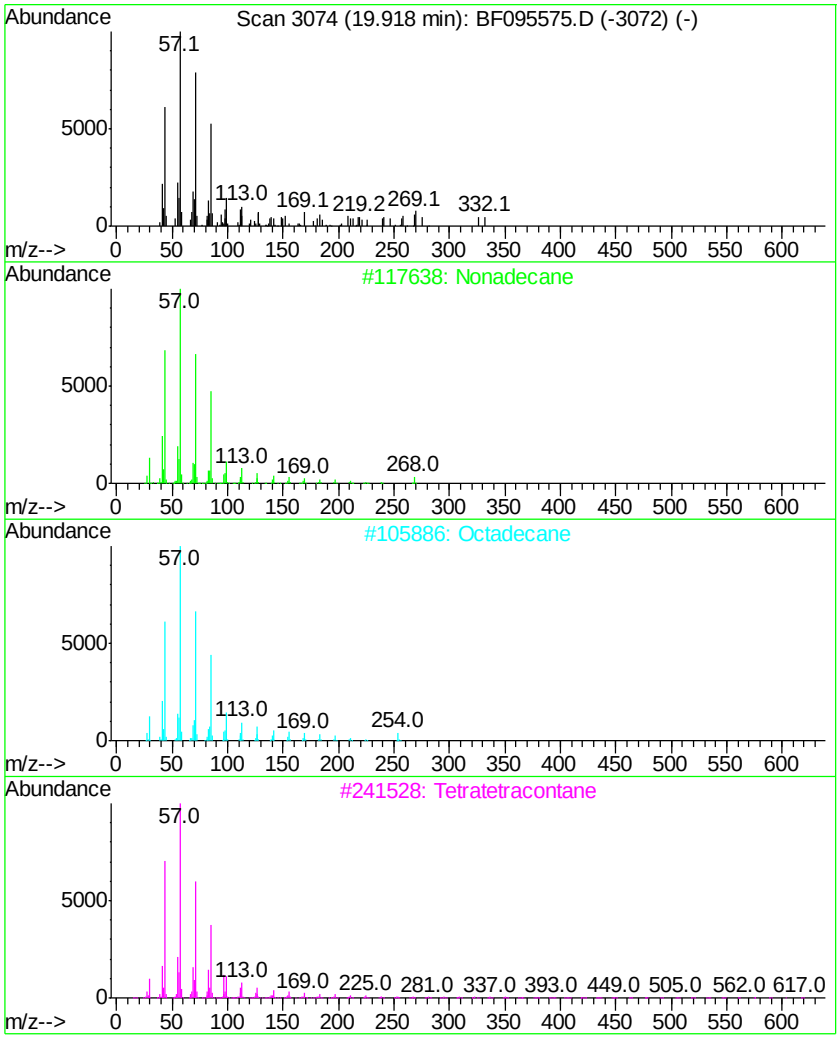
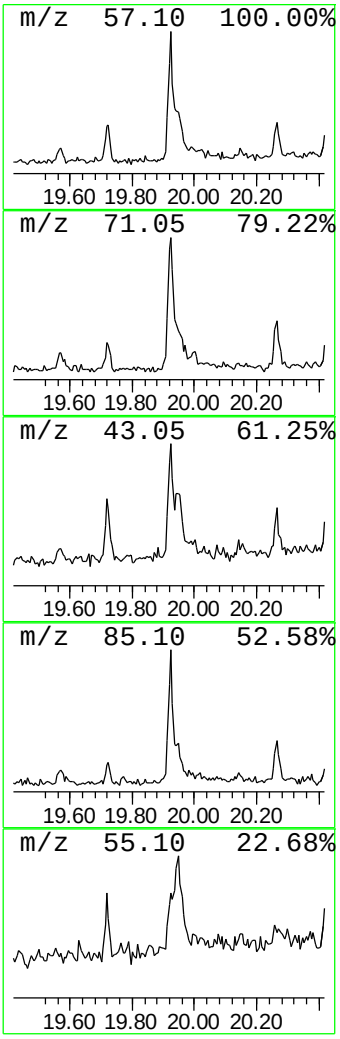
Peak Number 10 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.92	3.15 ng	77422	Perylene-d12	20.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Octadecane	254	C18H38	000593-45-3	93
3	Tetratetracontane	619	C44H90	007098-22-8	87
4	Hexatriacontane	507	C36H74	000630-06-8	80
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80





Library Search Compound Report

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Operator : SJ/MA
Sample : I3341-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM11-COMP-0-6

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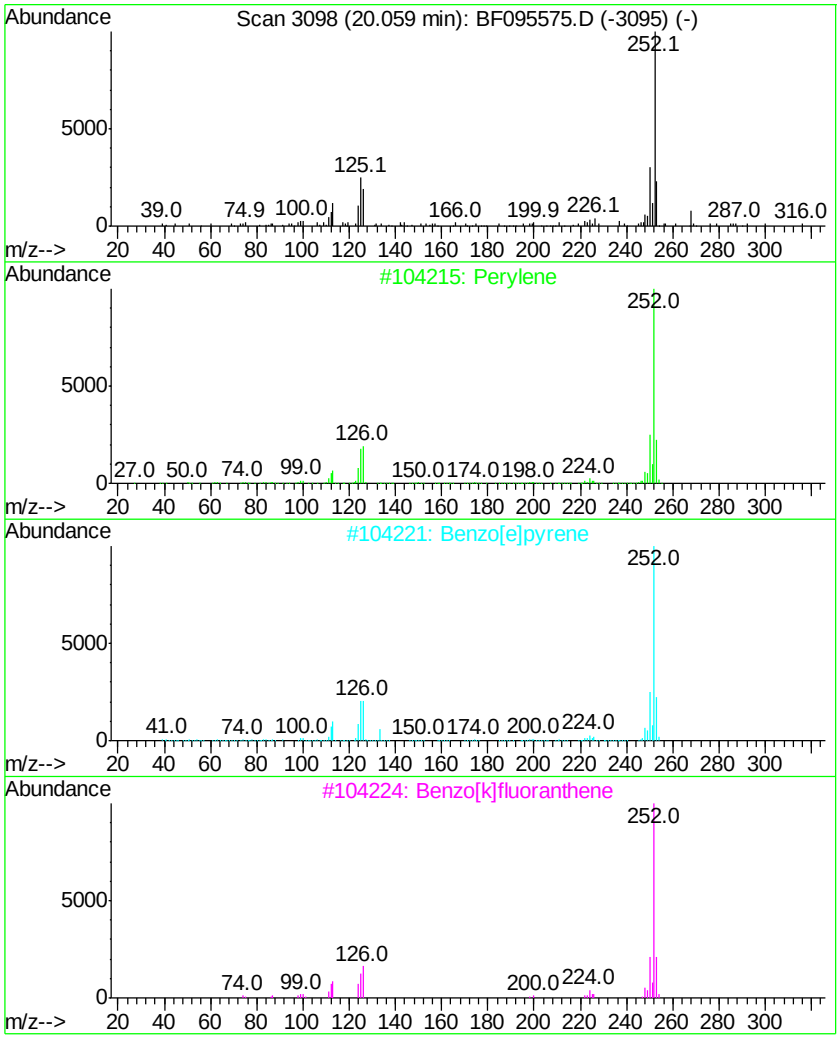
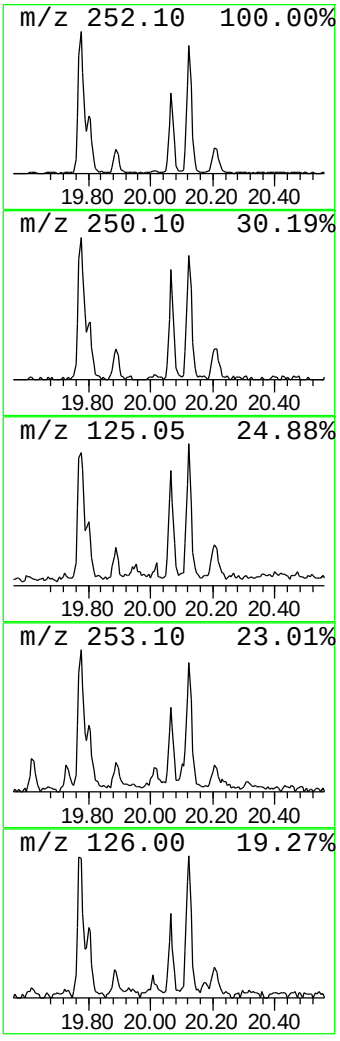
Peak Number 11 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.06	5.41 ng	133161	Perylene-d12	20.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	94
2	Benzo[e]pyrene	252	C20H12	000192-97-2	94
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93





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Acq On : 31 May 2017 21:12
Operator : SJ/MA
Sample : I3341-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM11-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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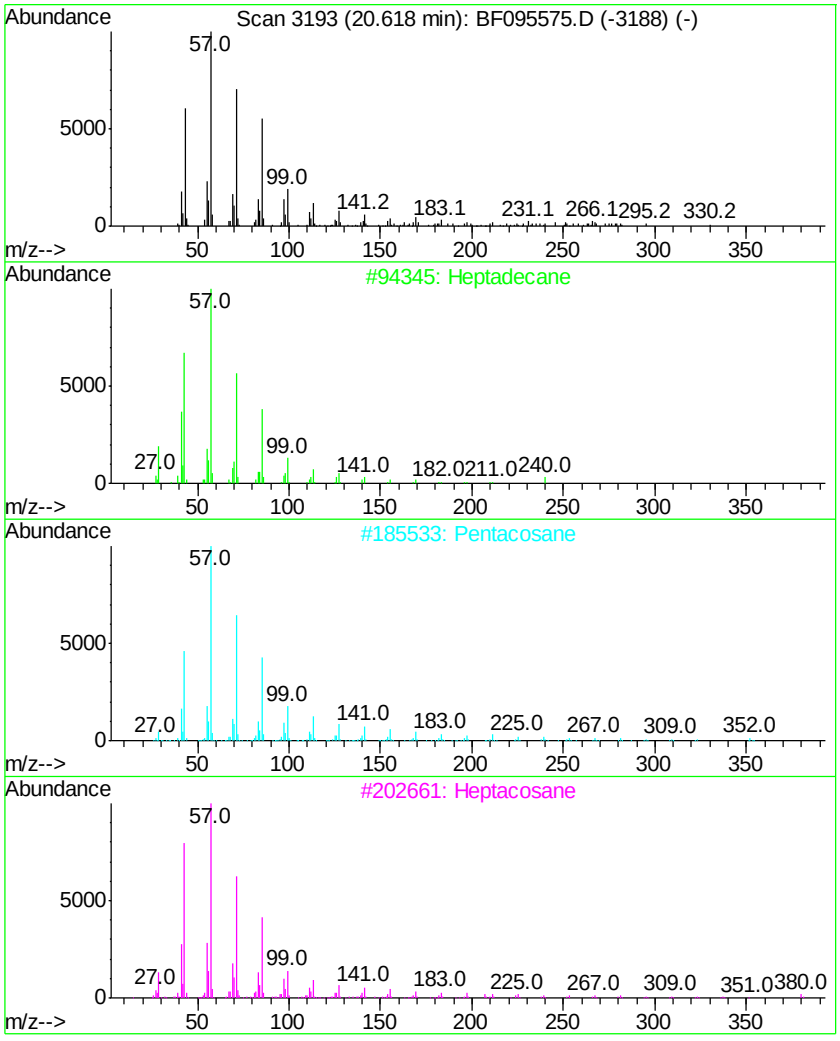
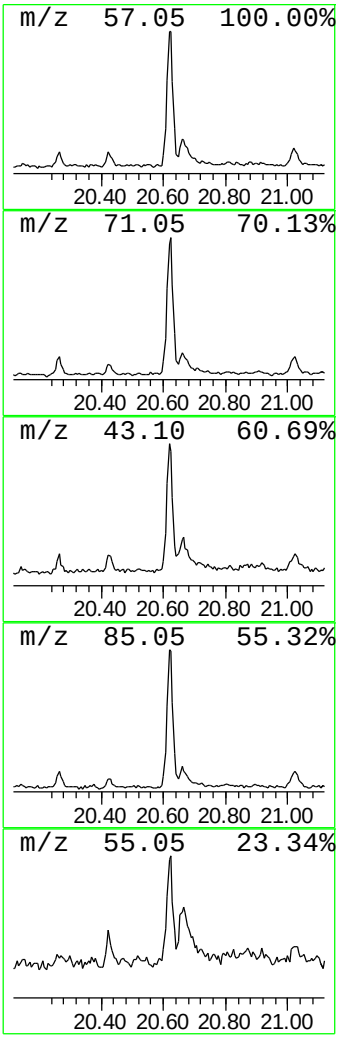
Peak Number 12 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.62	11.65 ng	286866	Perylene-d12	20.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Pentacosane	352	C25H52	000629-99-2	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5	2-methyloctacosane	408	C29H60	1000376-72-8	90





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Acq On : 31 May 2017 21:12
Operator : SJ/MA
Sample : I3341-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM11-COMP-0-6

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

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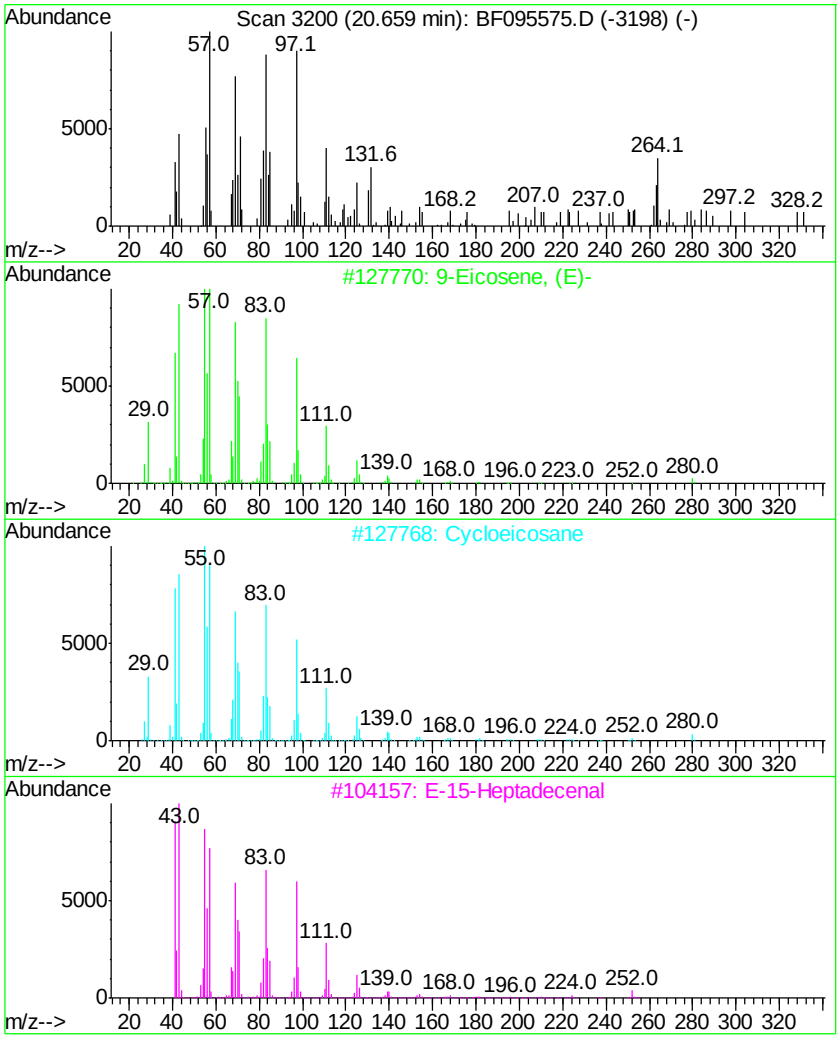
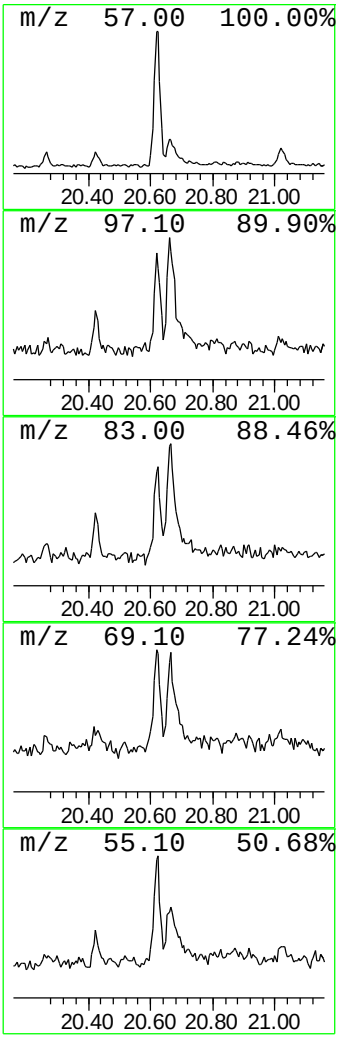
Peak Number 13 9-Eicosene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.66	5.22 ng	128491	Perylene-d12	20.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-	280	C20H40	074685-29-3	58
2	Cycloeicosane	280	C20H40	000296-56-0	49
3	E-15-Heptadecenal	252	C17H32O	1000130-97-9	45
4	Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	053907-60-1	45
5	Behenic alcohol	326	C22H46O	000661-19-8	42





Tentatively Identified Compound (LSC) summary

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Data File : BF095575.D
Acq On : 31 May 2017 21:12
Operator : SJ/MA
Sample : I3341-01
Misc :
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Instrument : BNA_F
ClientSampleId : NM11-COMP-0-6

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...	4.81	8.3	ng	227286	1	7.55	545515	20.0
unknown7.21	7.21	98.7	ng	2691440	1	7.55	545515	20.0
1-Dodecanethiol	15.32	2.7	ng	102537	4	14.81	766969	20.0
unknown15.74	15.74	2.5	ng	96912	4	14.81	766969	20.0
n-Hexadecanoic acid	15.80	7.1	ng	272799	4	14.81	766969	20.0
Pyrene, 2-methyl-	17.51	2.2	ng	91193	5	18.50	829243	20.0
1-Heneicosanol	18.40	4.0	ng	165279	5	18.50	829243	20.0
14-Heptadecenal	19.72	2.7	ng	66700	6	20.18	492273	20.0
Nonadecane	19.92	3.1	ng	77422	6	20.18	492273	20.0
Perylene	20.06	5.4	ng	133161	6	20.18	492273	20.0
Heptadecane	20.62	11.7	ng	286866	6	20.18	492273	20.0
9-Eicosene, (E)-	20.66	5.2	ng	128491	6	20.18	492273	20.0