LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095579.D
Acq On : 31 May 2017 23:21
Operator : SJ/MA
Sample : I3341-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-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	4.807	502	505	519	rBV	79870	194655	9.00%	1.007%
2	5.472	614	618	650	rBV	988874	1928768	89.21%	9.983%
3	7.107	892	896	910	rBV	1157328	1803435	83.41%	9.334%
4	7.213	910	914	930	rVB	1454387	2162051	100.00%	11.190%
5	7.554	968	972	983	rBV	383879	490591	22.69%	2.539%
6	7.789	1007	1012	1029	rBV	1175432	1517522	70.19%	7.854%
7	8.466	1122	1127	1157	rBV	801855	1171160	54.17%	6.062%
8	9.583	1313	1317	1329	rBV	494957	655839	30.33%	3.394%
9	11.360	1613	1619	1631	rBV	1679919	2076058	96.02%	10.745%
10	12.048	1732	1736	1748	rBV	324195	398702	18.44%	2.064%
11	12.407	1792	1797	1806	rBV2	617359	818549	37.86%	4.237%
12	13.254	1933	1941	1946	rBV2	40381	49404	2.29%	0.256%
13	13.707	2013	2018	2034	rBV	806333	1129500	52.24%	5.846%
14	14.024	2068	2072	2083	rBV	38832	60579	2.80%	0.314%
15	14.759	2192	2197	2201	rBV	27662	34111	1.58%	0.177%
16	14.812	2201	2206	2210	rVV	469773	601882	27.84%	3.115%
17	14.848	2210	2212	2219	rVB	61669	83826	3.88%	0.434%
18	15.736	2360	2363	2365	rBV2	28219	32078	1.48%	0.166%
19	15.801	2370	2374	2381	rVB2	136785	173360	8.02%	0.897%
20	16.612	2508	2512	2523	rVV	153825	171874	7.95%	0.890%
21	16.695	2523	2526	2531	rVB2	32998	34353	1.59%	0.178%
22	16.895	2556	2560	2561	rBV	30007	34143	1.58%	0.177%
23	16.918	2561	2564	2573	rVB	141551	167920	7.77%	0.869%
24	17.153	2600	2604	2612	rVB	957564	1073034	49.63%	5.554%
25	17.518	2662	2666	2669	rVV3	21114	30779	1.42%	0.159%
26	17.853	2720	2723	2728	rVB2	20153	24137	1.12%	0.125%
27	17.989	2739	2746	2753	rBV4	37676	57978	2.68%	0.300%
28	18.136	2766	2771	2774	rBV2	28562	29250	1.35%	0.151%
29	18.400	2812	2816	2825	rBV2	101967	164621	7.61%	0.852%
30	18.506	2825	2834	2838	rBV2	534370	717194	33.17%	3.712%
31	18.542	2838	2840	2842	rVV	32631	26584	1.23%	0.138%
32	18.812	2881	2886	2891	rBV5	20128	34667	1.60%	0.179%
33	19.018	2915	2921	2924	rBV3	19358	33052	1.53%	0.171%
34	19.206	2949	2953	2960	rBV7	34198	56250	2.60%	0.291%

LSC Area Percent Report

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Data File : BF095579.D
Acq On : 31 May 2017 23:21
Operator : SJ/MA
Sample : I3341-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-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

35	19.530	3004	3008	3013	rBV8	13418	26380	1.22%	0.137%
36	19.636	3020	3026	3029	rBV3	27826	40517	1.87%	0.210%
37	19.724	3038	3041	3045	rBV4	23973	29085	1.35%	0.151%
38	19.777	3047	3050	3053	rBV	99750	130564	6.04%	0.676%
39	19.924	3072	3075	3078	rBV2	44142	53576	2.48%	0.277%
40	20.071	3096	3100	3104	rVB	57917	76272	3.53%	0.395%
41	20.124	3106	3109	3114	rBV	83780	108863	5.04%	0.563%
42	20.177	3114	3118	3129	rVB	419701	526109	24.33%	2.723%
43	20.430	3158	3161	3165	rBV3	30957	38976	1.80%	0.202%
44	20.624	3189	3194	3197	rBV	90203	126001	5.83%	0.652%
45	20.665	3198	3201	3209	rVB6	40156	72766	3.37%	0.377%
46	21.030	3260	3263	3265	rBV4	18335	23079	1.07%	0.119%
47	21.436	3329	3332	3336	rBV2	24067	30574	1.41%	0.158%

Sum of corrected areas: 19320668

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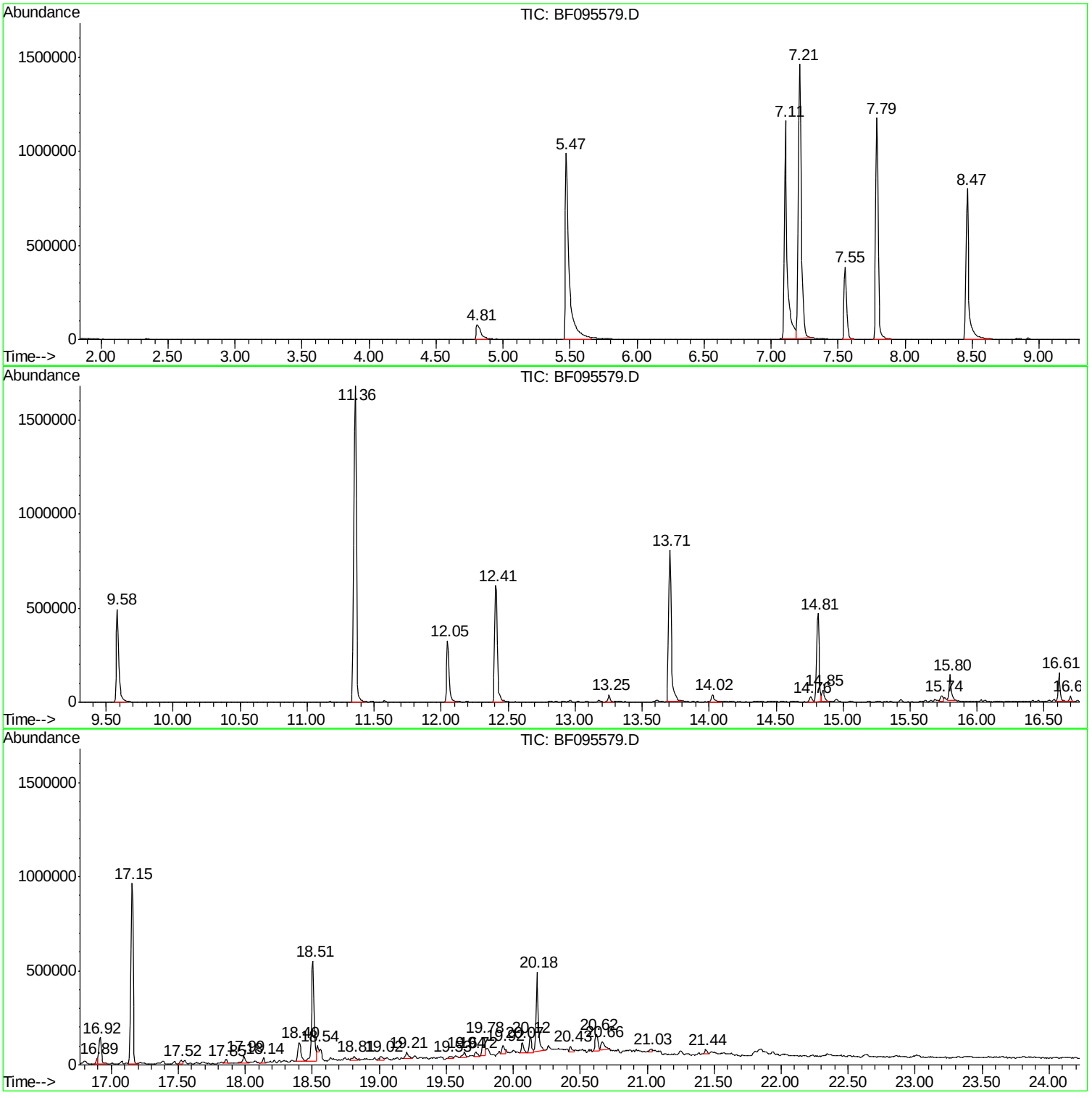
Instrument :
BNA_F
ClientSampleId :
NM1-COMP-0-6

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095579.D
Acq On : 31 May 2017 23:21
Operator : SJ/MA
Sample : I3341-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-0-6

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

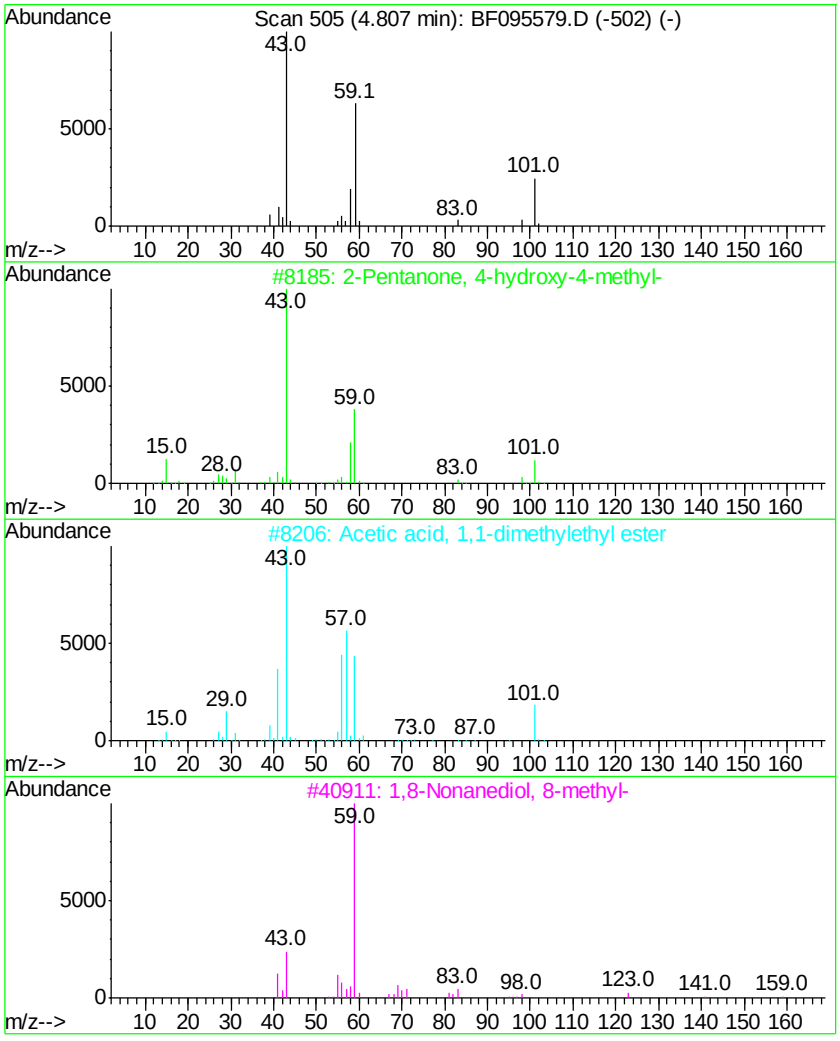
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

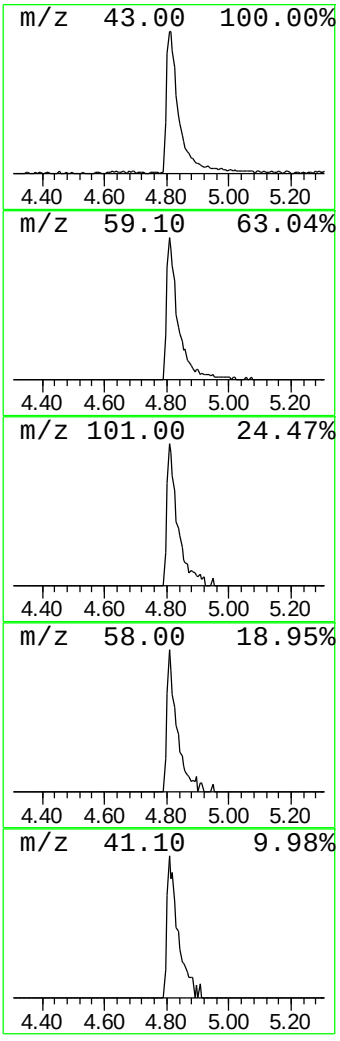
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	7.94 ng	194655	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	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
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Acq On : 31 May 2017 23:21
Operator : SJ/MA
Sample : I3341-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-0-6

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

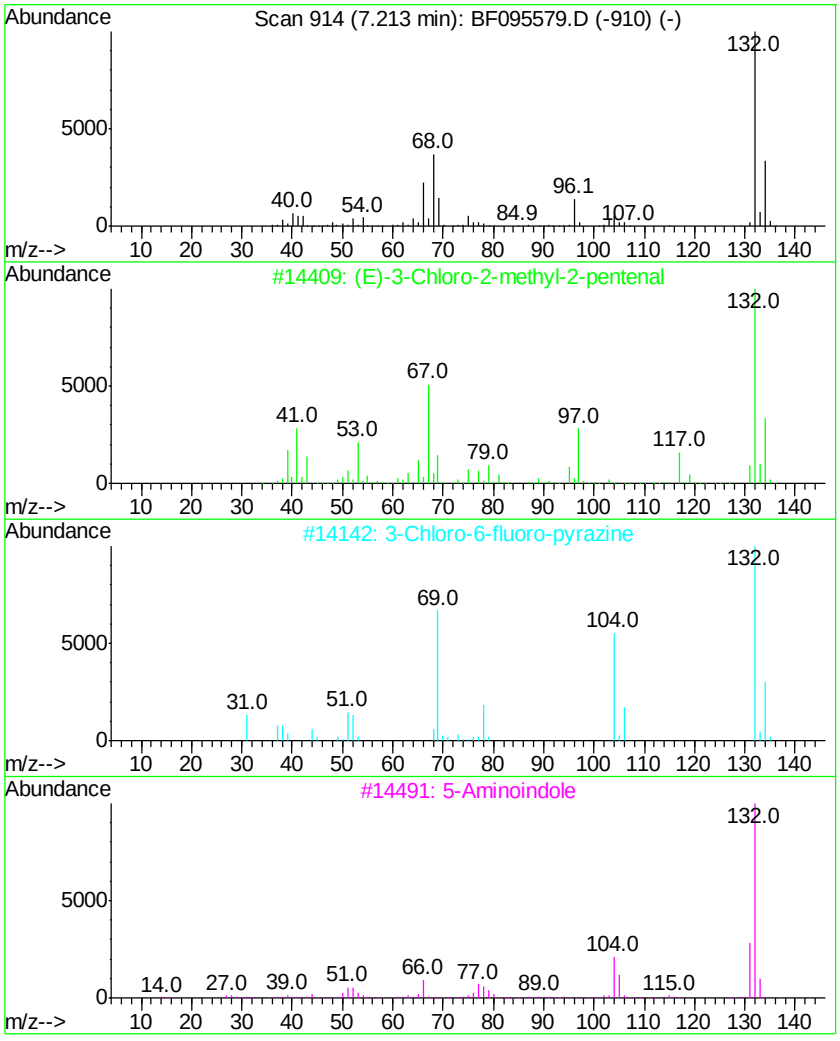
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

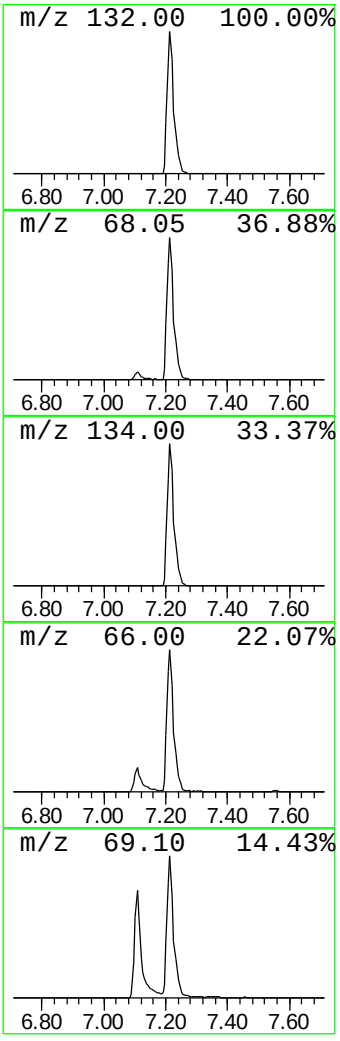
****

Peak Number 2 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	88.14 ng	2162050	1,4-Dichlorobenzene-d4	7.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
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Operator : SJ/MA
Sample : I3341-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-0-6

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

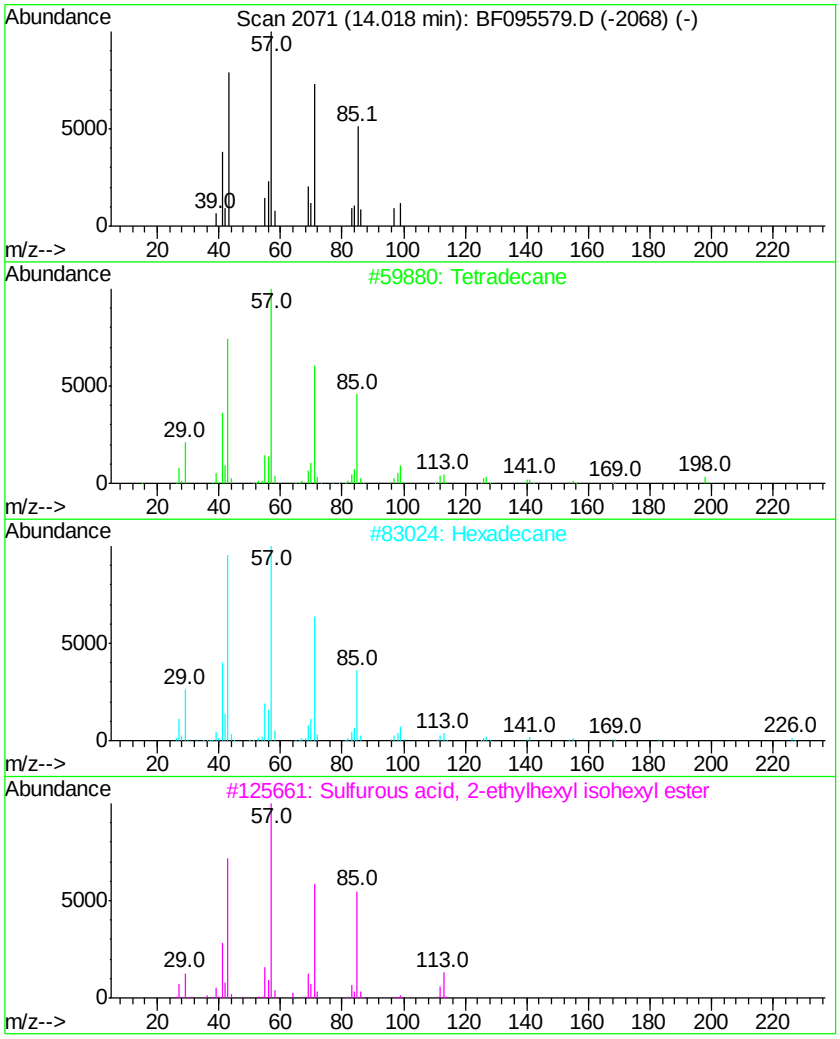
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

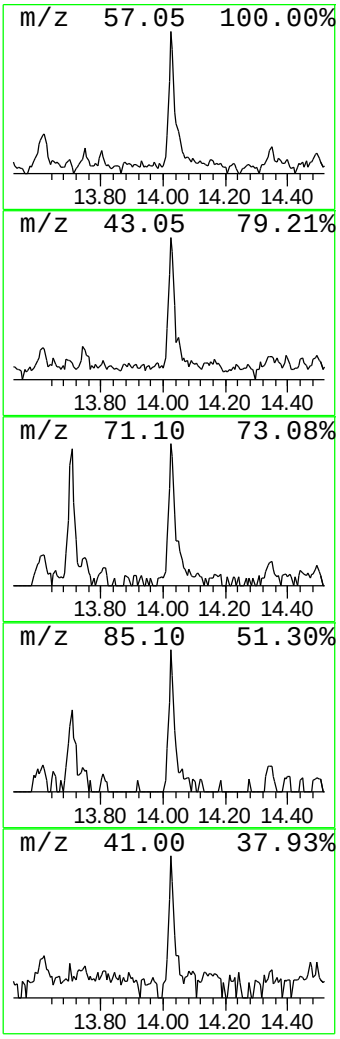
****

Peak Number 4 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.02	2.01 ng	60579	Phenanthrene-d10	14.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	80
2	Hexadecane	226	C16H34	000544-76-3	72
3	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72
4	Sulfurous acid, hexyl heptyl ester	264	C13H28O3S	1000309-12-9	58
5	Sulfurous acid, isohexyl 2-penty...	236	C11H24O3S	1000309-15-5	53





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Sample : I3341-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-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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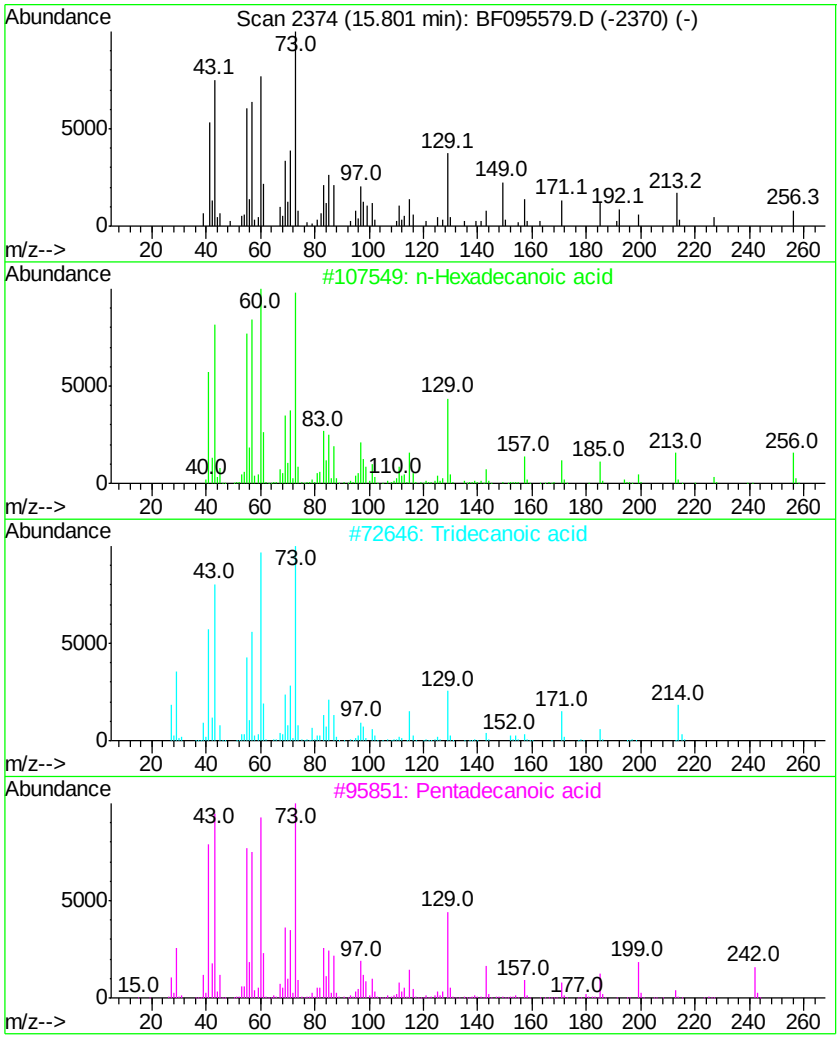
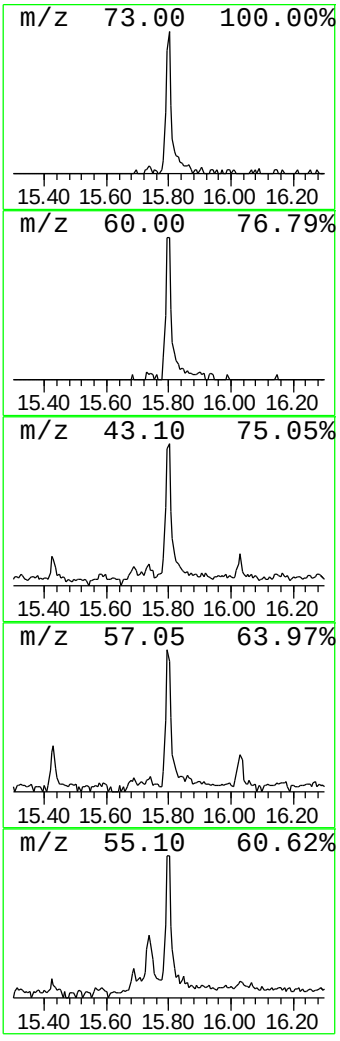
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	5.76 ng	173360	Phenanthrene-d10	14.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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Operator : SJ/MA
Sample : I3341-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-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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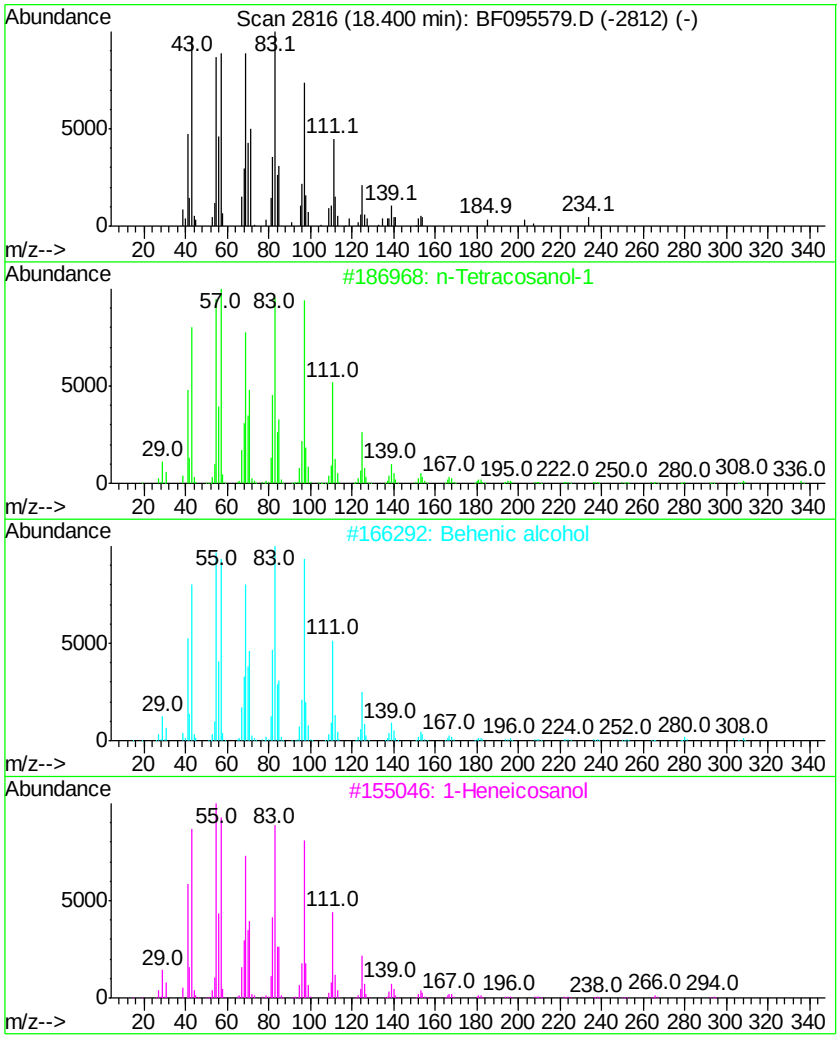
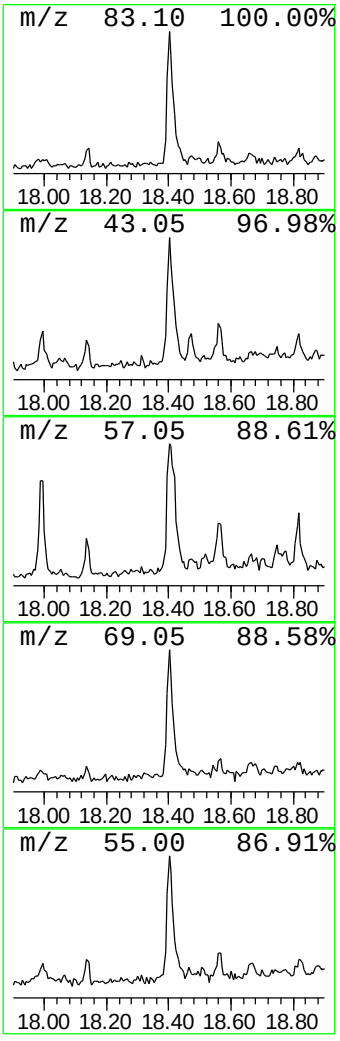
Peak Number 6 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	4.59 ng	164621	Chrysene-d12	18.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Octacosanol	410	C28H58O	000557-61-9	93
5	1-Heptacosanol	396	C27H56O	002004-39-9	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095579.D
Acq On : 31 May 2017 23:21
Operator : SJ/MA
Sample : I3341-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-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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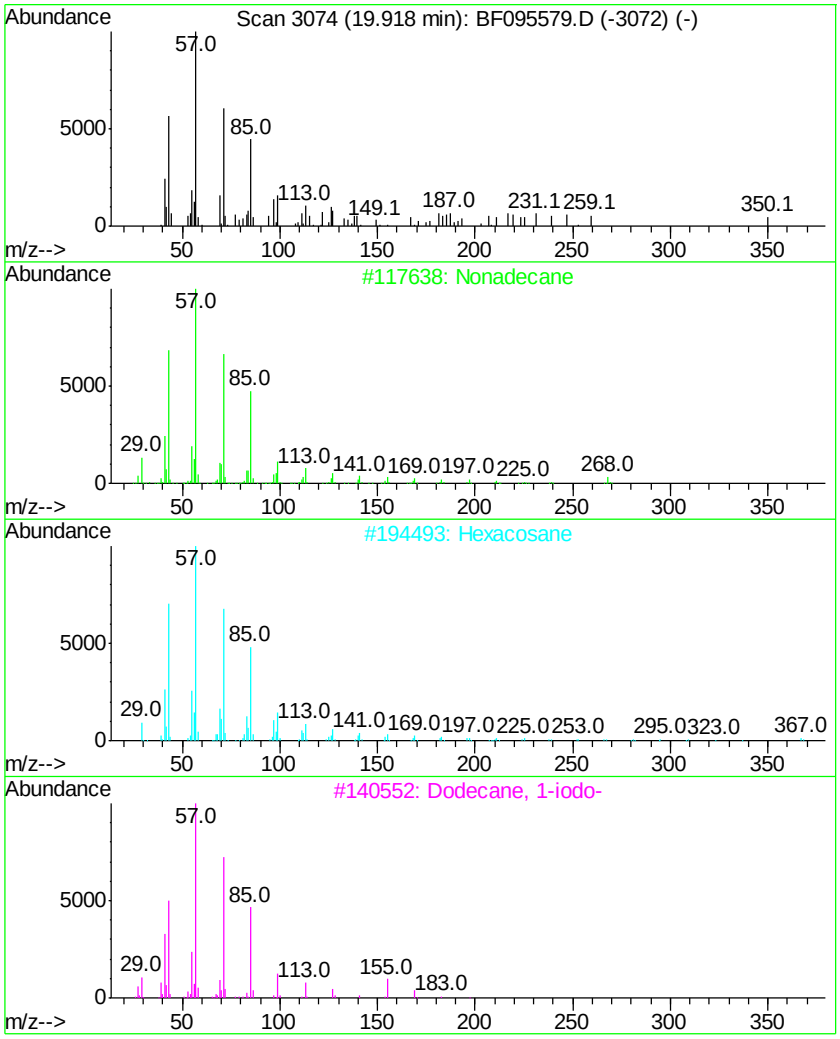
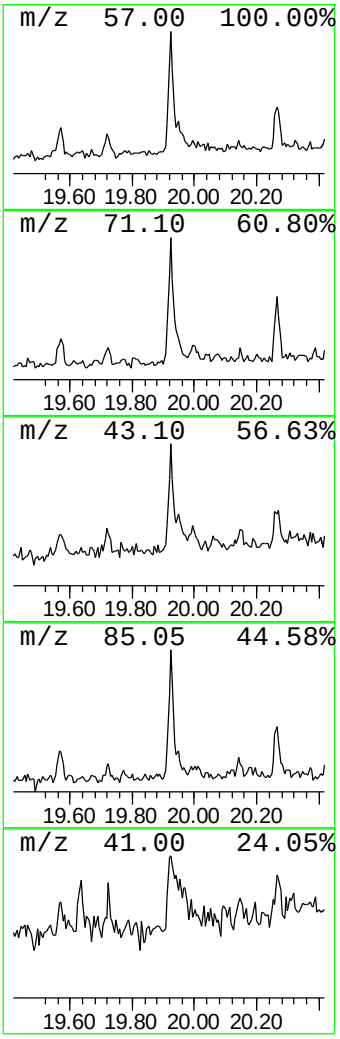
Peak Number 7 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.92	2.04 ng	53576	Perylene-d12	20.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Hexacosane	366	C26H54	000630-01-3	83
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
4	Triacontane	422	C30H62	000638-68-6	80
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	80





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Instrument : BNA_F
ClientSampleId : NM1-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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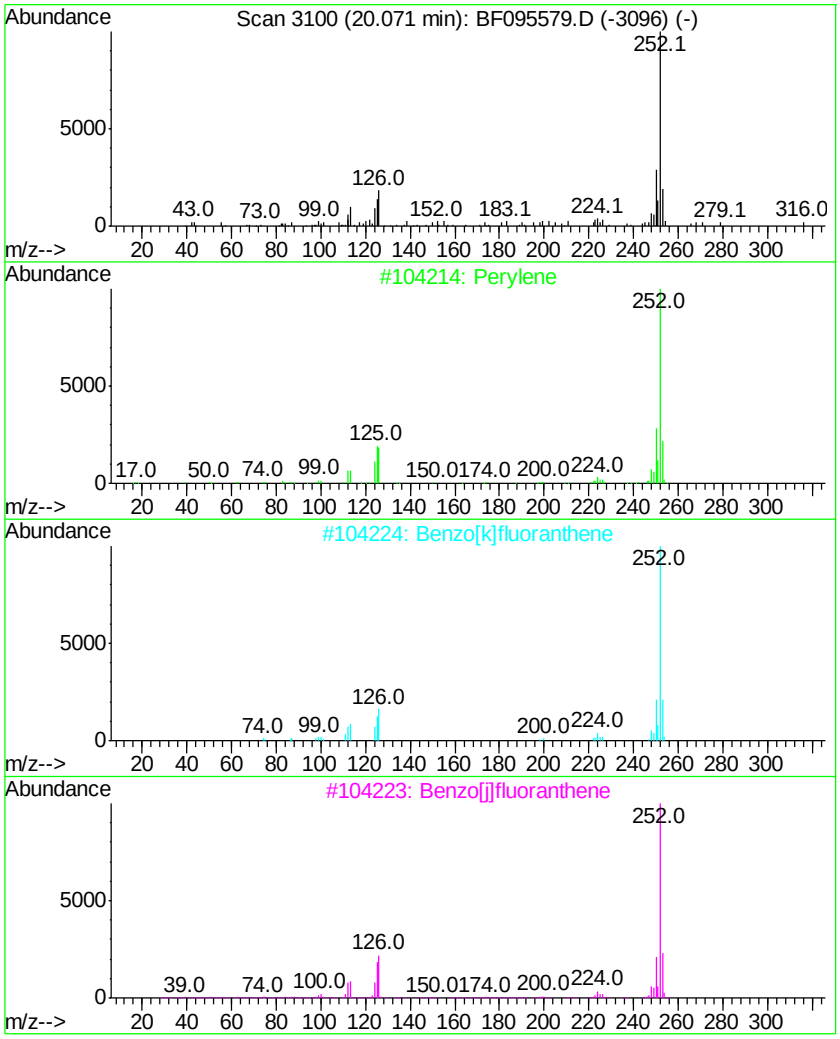
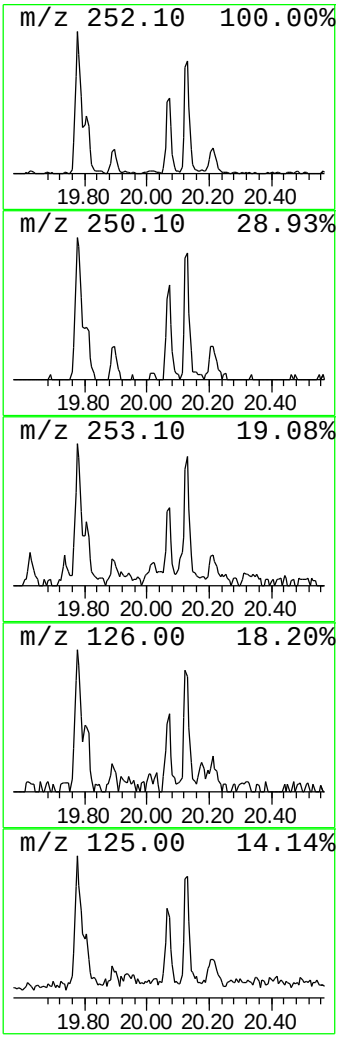
Peak Number 8 Perylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.07	2.90 ng	76272	Perylene-d12	20.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
4	Benzo[e]pyrene	252	C20H12	000192-97-2	96
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095579.D
Acq On : 31 May 2017 23:21
Operator : SJ/MA
Sample : I3341-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-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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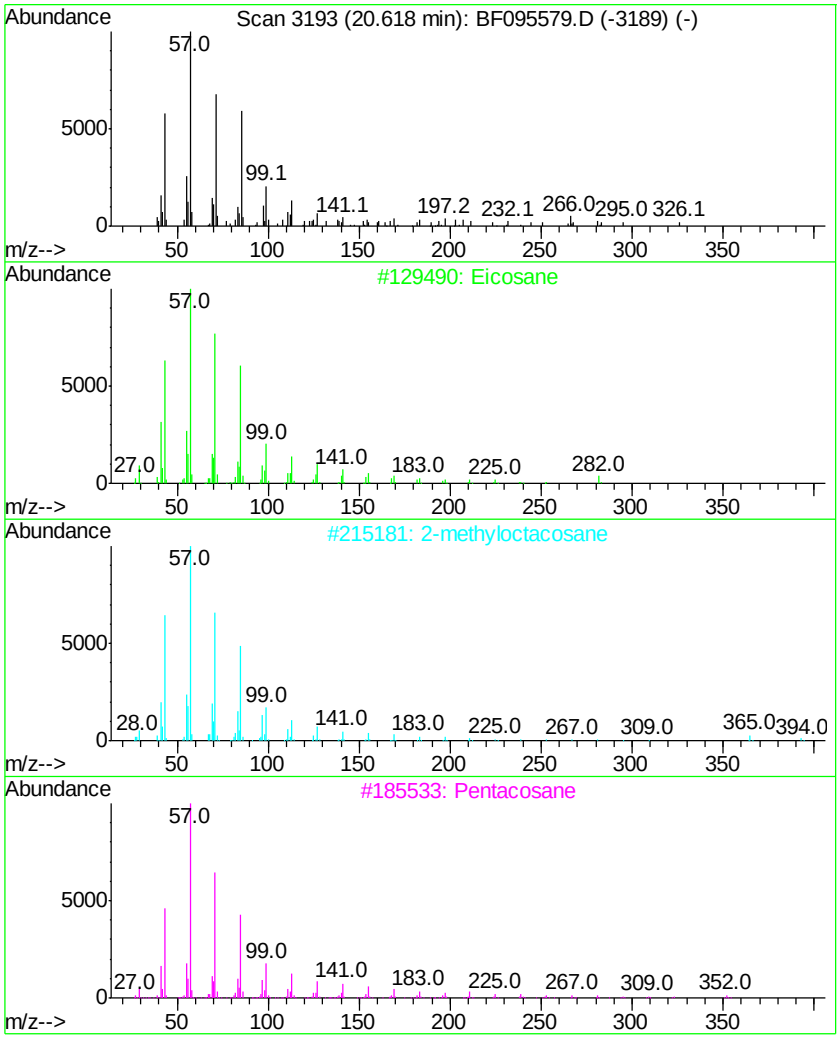
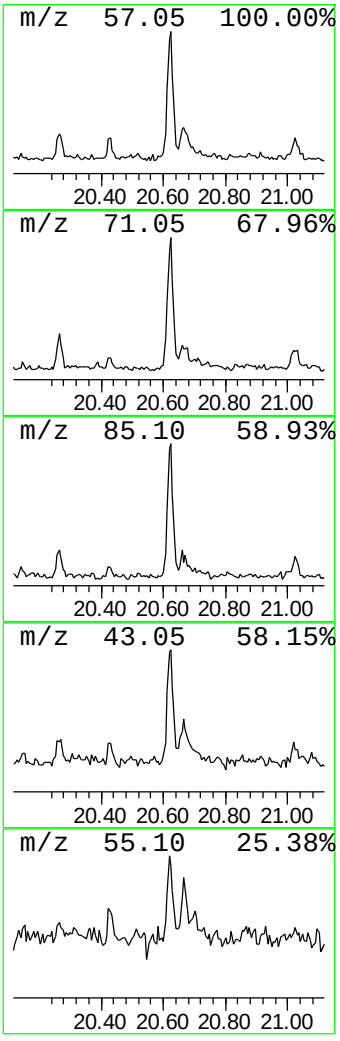
Peak Number 9 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.62	4.79 ng	126001	Perylene-d12	20.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	2-methyloctacosane	408	C29H60	1000376-72-8	86
3	Pentacosane	352	C25H52	000629-99-2	86
4	Tridecane, 3-methyl-	198	C14H30	006418-41-3	83
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095579.D
Acq On : 31 May 2017 23:21
Operator : SJ/MA
Sample : I3341-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-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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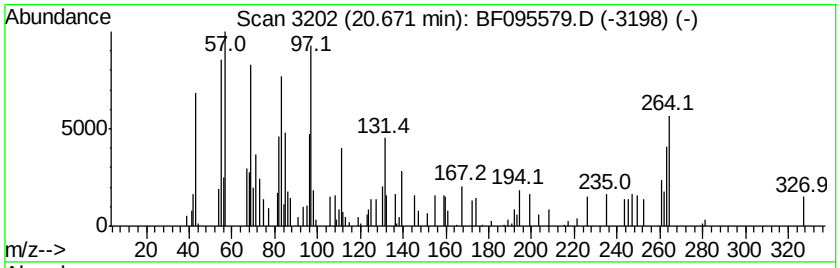
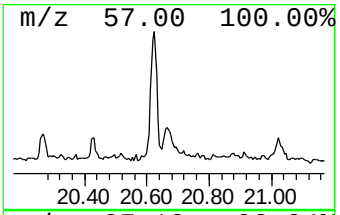
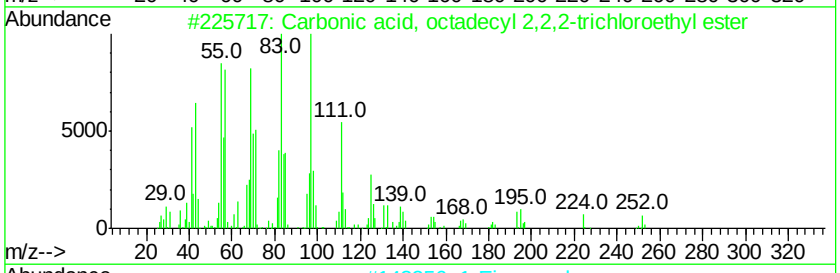
Peak Number 10 unknown20.67 Concentration Rank 8

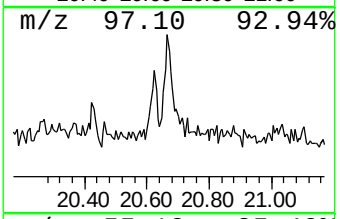
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.67	2.77 ng	72766	Perylene-d12	20.18

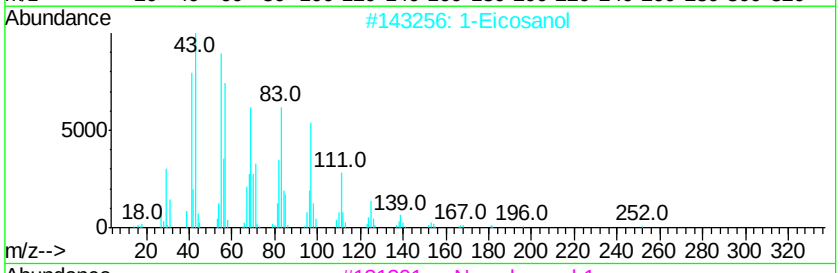
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	49
2	1-Eicosanol	298	C20H42O	000629-96-9	49
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	49
4	E-15-Heptadecenal	252	C17H32O	1000130-97-9	47
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	41

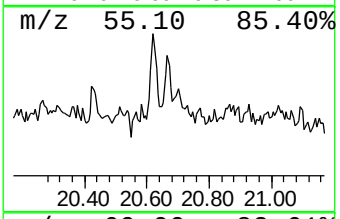


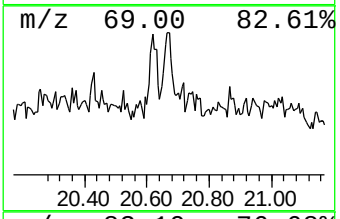


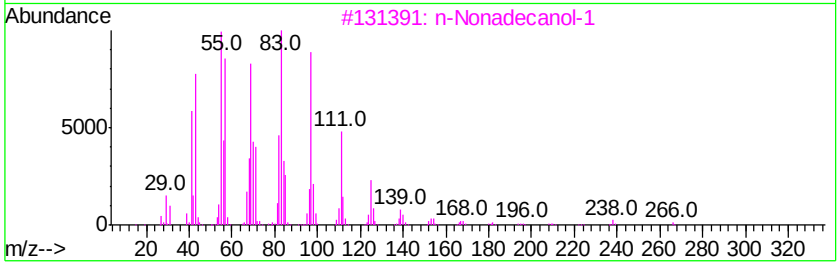


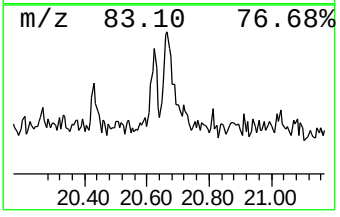












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095579.D
Acq On : 31 May 2017 23:21
Operator : SJ/MA
Sample : I3341-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-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	7.9	ng	194655	1	7.55	490591	20.0
unknown7.21	7.21	88.1	ng	2162050	1	7.55	490591	20.0
Tetradecane	14.02	2.0	ng	60579	4	14.81	601882	20.0
n-Hexadecanoic acid	15.80	5.8	ng	173360	4	14.81	601882	20.0
n-Tetracosanol-1	18.40	4.6	ng	164621	5	18.51	717194	20.0
Nonadecane	19.92	2.0	ng	53576	6	20.18	526109	20.0
Perylene	20.07	2.9	ng	76272	6	20.18	526109	20.0
Eicosane	20.62	4.8	ng	126001	6	20.18	526109	20.0
unknown20.67	20.67	2.8	ng	72766	6	20.18	526109	20.0