LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095520.D
Acq On : 28 May 2017 3:42
Operator : SJ/MA
Sample : I3244-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM8-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	5.096	533	537	556	rBV	78212	201070	9.13%	1.068%
2	5.701	637	640	680	rBV	622233	1816075	82.45%	9.648%
3	7.284	906	909	925	rBV	660818	1635835	74.27%	8.690%
4	7.401	925	929	950	rVB	1222849	2202582	100.00%	11.701%
5	7.737	982	986	1001	rVB	431218	554722	25.19%	2.947%
6	7.972	1021	1026	1042	rBV	1195231	1554765	70.59%	8.259%
7	8.642	1136	1140	1163	rBV	439063	1041716	47.30%	5.534%
8	9.766	1327	1331	1358	rBV	289862	708488	32.17%	3.764%
9	11.530	1626	1631	1654	rBV	937087	1805458	81.97%	9.591%
10	12.242	1748	1752	1769	rBV	85036	178727	8.11%	0.949%
11	12.595	1807	1812	1831	rBV2	386087	724427	32.89%	3.848%
12	13.424	1949	1953	1959	rBV	23831	28722	1.30%	0.153%
13	13.901	2029	2034	2061	rBV	390853	848491	38.52%	4.507%
14	14.195	2079	2084	2095	rBV2	20746	34777	1.58%	0.185%
15	15.001	2217	2221	2226	rVV	288710	459967	20.88%	2.443%
16	15.036	2226	2227	2241	rVB	102075	182808	8.30%	0.971%
17	15.489	2296	2304	2311	rBV3	24222	59480	2.70%	0.316%
18	15.848	2360	2365	2370	rVV2	14084	23897	1.08%	0.127%
19	15.948	2378	2382	2395	rVB4	45167	102745	4.66%	0.546%
20	16.783	2520	2524	2533	rBV	220365	312957	14.21%	1.663%
21	16.854	2533	2536	2543	rVB	23001	27013	1.23%	0.144%
22	17.089	2571	2576	2585	rBV	250519	333445	15.14%	1.771%
23	17.312	2610	2614	2625	rVV	1017879	1229255	55.81%	6.530%
24	17.412	2627	2631	2640	rVB4	16174	31744	1.44%	0.169%
25	17.554	2652	2655	2662	rVB2	24407	37225	1.69%	0.198%
26	17.642	2666	2670	2674	rBV2	19348	25107	1.14%	0.133%
27	17.695	2674	2679	2683	rBV3	26831	39429	1.79%	0.209%
28	18.389	2794	2797	2800	rVV2	22258	23451	1.06%	0.125%
29	18.553	2817	2825	2832	rBV8	27947	83272	3.78%	0.442%
30	18.671	2839	2845	2849	rBV2	495615	765542	34.76%	4.067%
31	18.706	2849	2851	2862	rVV2	143064	244323	11.09%	1.298%
32	18.801	2864	2867	2875	rVB2	27998	45156	2.05%	0.240%
33	19.189	2930	2933	2936	rVB	20868	22961	1.04%	0.122%
34	19.301	2944	2952	2955	rBV9	16259	35489	1.61%	0.189%

LSC Area Percent Report

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Acq On : 28 May 2017 3:42
Operator : SJ/MA
Sample : I3244-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM8-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	19.342	2955	2959	2962	rBV6	20785	28222	1.28%	0.150%
36	19.706	3018	3021	3026	rVB7	14482	24090	1.09%	0.128%
37	19.783	3030	3034	3041	rVB3	33460	53638	2.44%	0.285%
38	19.859	3041	3047	3053	rBV8	25544	40548	1.84%	0.215%
39	19.948	3059	3062	3065	rBV	128183	180297	8.19%	0.958%
40	20.065	3078	3082	3085	rBV	69090	78463	3.56%	0.417%
41	20.242	3108	3112	3117	rBV	81850	96457	4.38%	0.512%
42	20.300	3118	3122	3127	rBV	100078	129012	5.86%	0.685%
43	20.353	3127	3131	3139	rBV	298001	465275	21.12%	2.472%
44	20.530	3156	3161	3164	rBV7	12544	23952	1.09%	0.127%
45	20.789	3201	3205	3210	rBV	77485	97806	4.44%	0.520%
46	20.883	3219	3221	3226	rVB6	18837	22593	1.03%	0.120%
47	21.712	3357	3362	3369	rVB4	51814	105588	4.79%	0.561%
48	22.100	3424	3428	3434	rBV2	27997	57101	2.59%	0.303%

Sum of corrected areas: 18824163

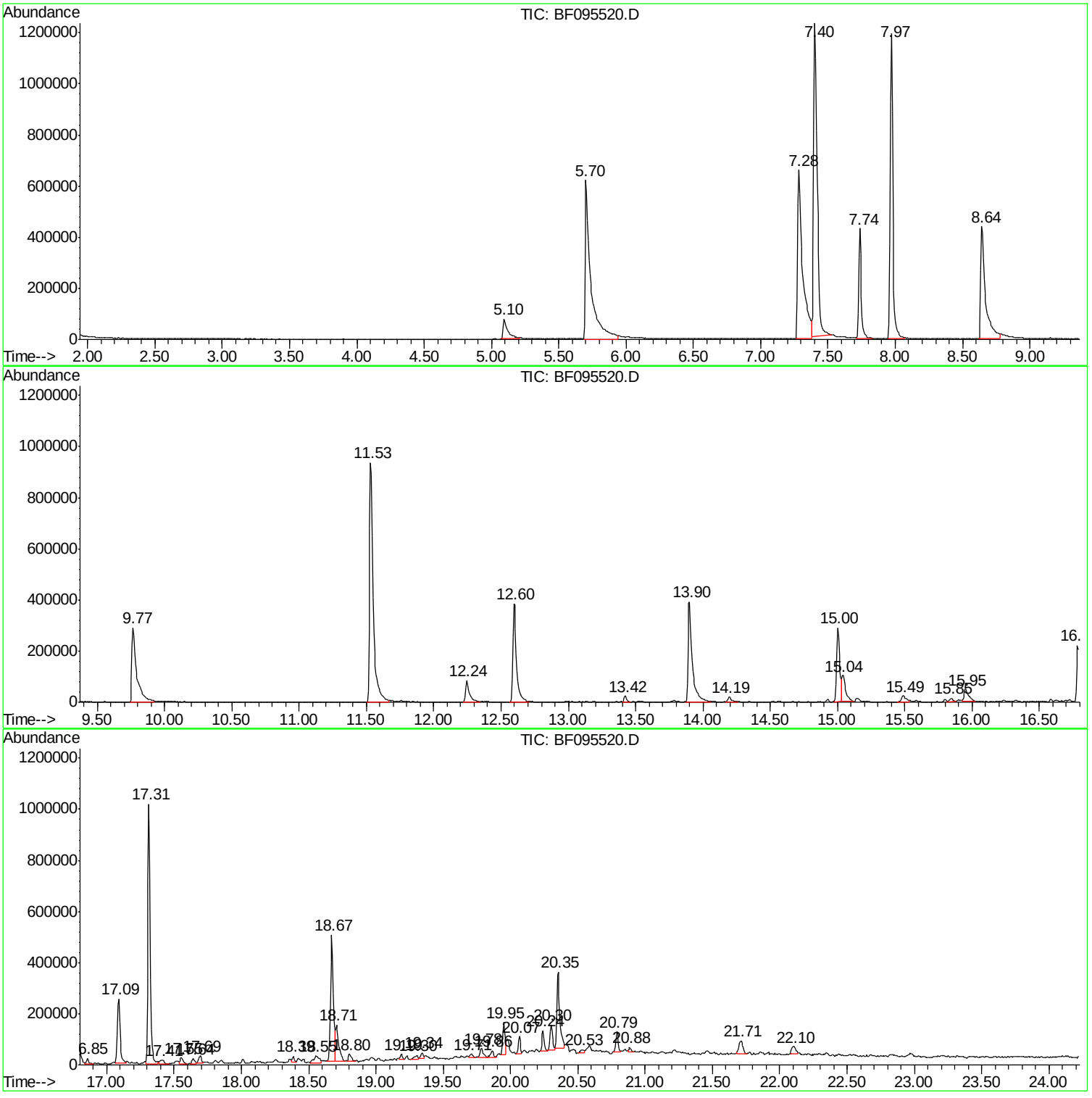
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095520.D
Acq On : 28 May 2017 3:42
Operator : SJ/MA
Sample : I3244-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM8-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\BF052717\
Data File : BF095520.D
Acq On : 28 May 2017 3:42
Operator : SJ/MA
Sample : I3244-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM8-COMP-0-6

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

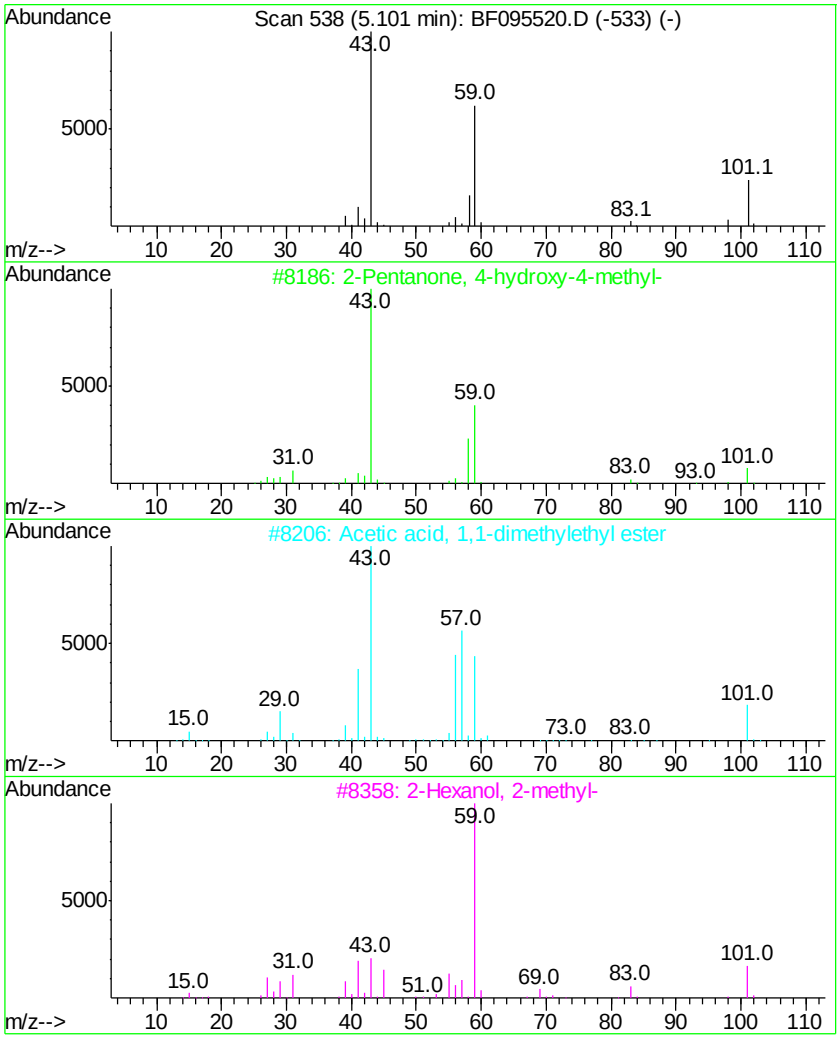
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

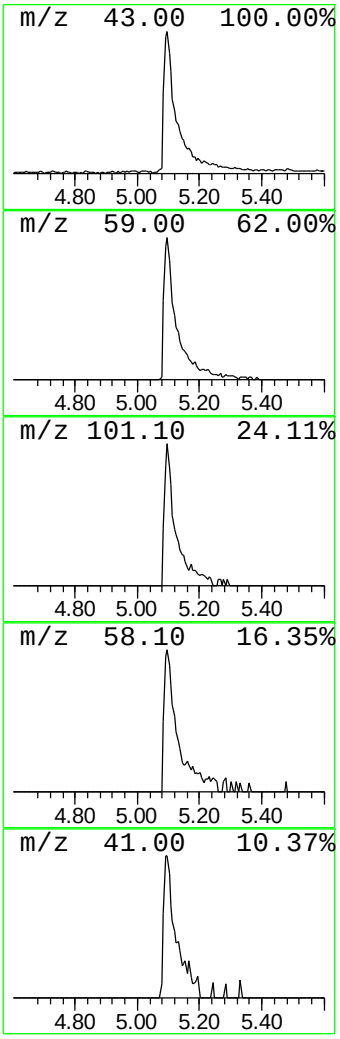
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	7.25 ng	201070	1,4-Dichlorobenzene-d4	7.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4	3-Hexanol	102	C6H14O	000623-37-0	25
5	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095520.D
Acq On : 28 May 2017 3:42
Operator : SJ/MA
Sample : I3244-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM8-COMP-0-6

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

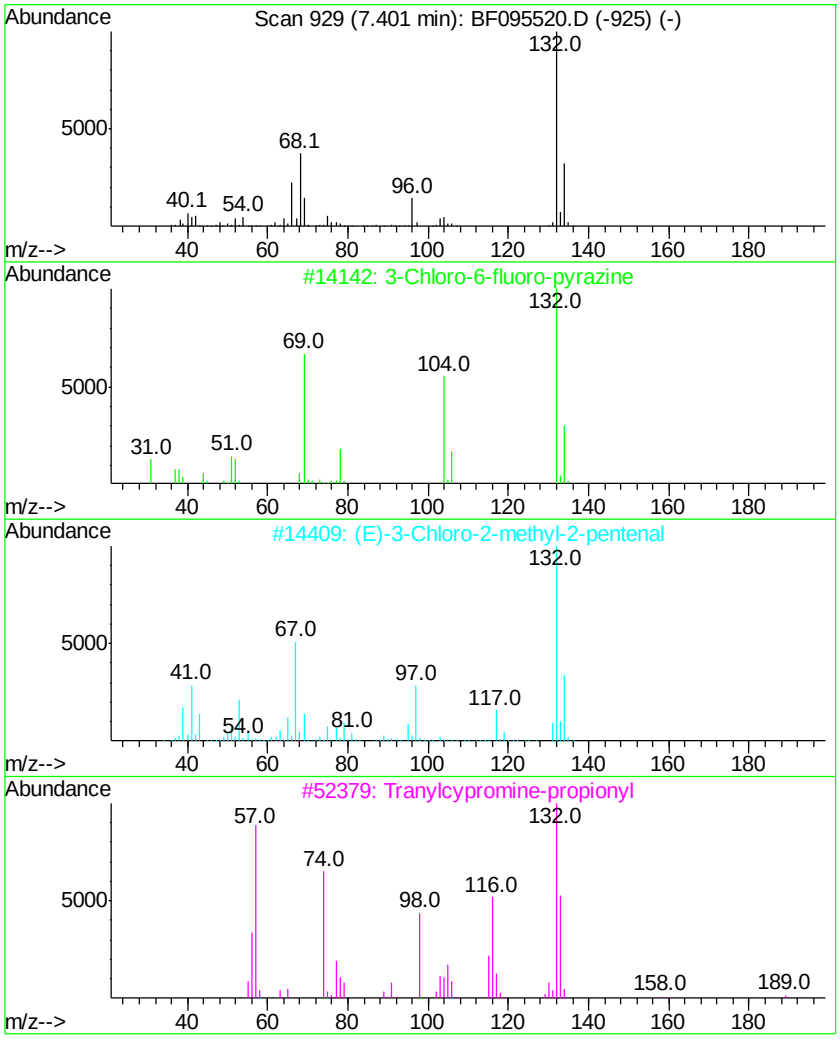
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

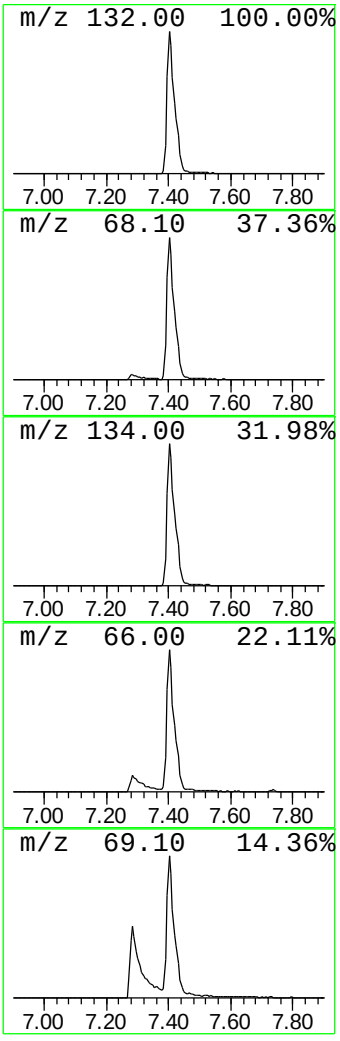
****

Peak Number 2 unknown7.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	79.41 ng	2202580	1,4-Dichlorobenzene-d4	7.74

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	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095520.D
Acq On : 28 May 2017 3:42
Operator : SJ/MA
Sample : I3244-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM8-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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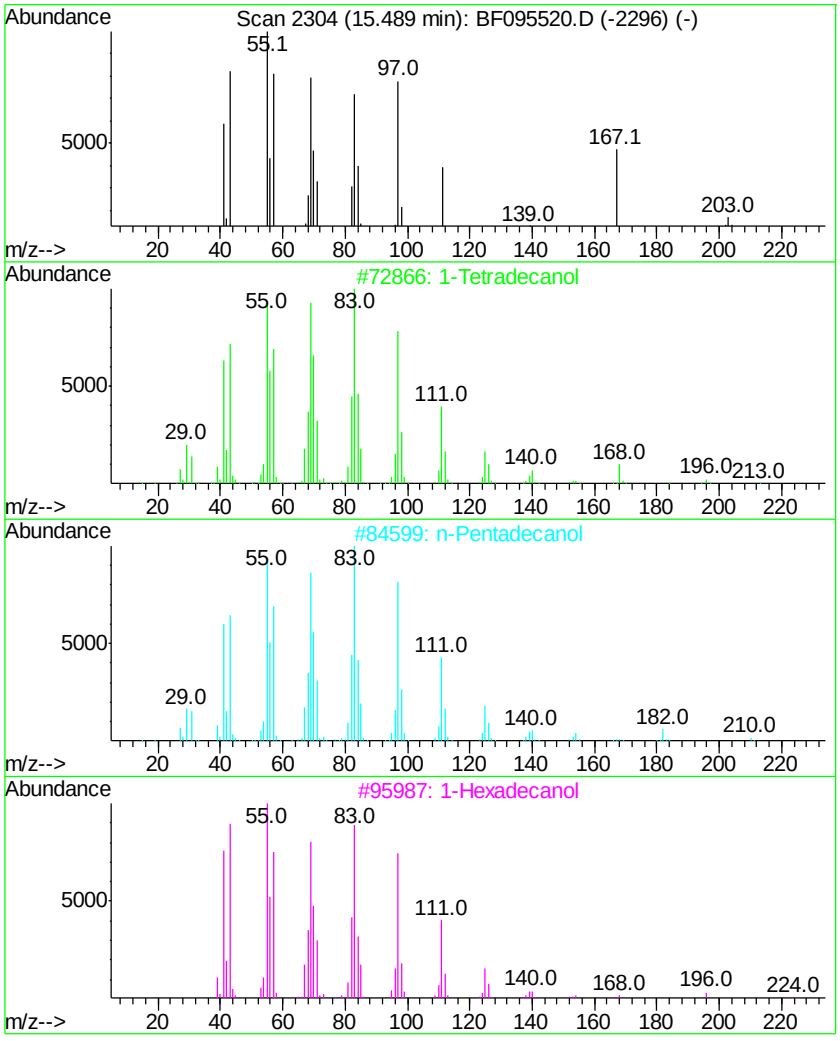
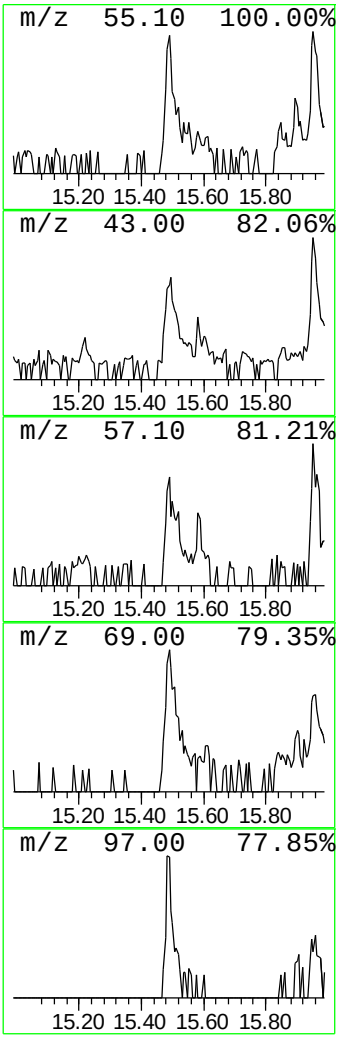
Peak Number 4 1-Tetradecanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.49	2.59 ng	59480	Phenanthrene-d10	15.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecanol	214	C14H30O	000112-72-1	87
2	n-Pentadecanol	228	C15H32O	000629-76-5	87
3	1-Hexadecanol	242	C16H34O	036653-82-4	81
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	81
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
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Operator : SJ/MA
Sample : I3244-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM8-COMP-0-6

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

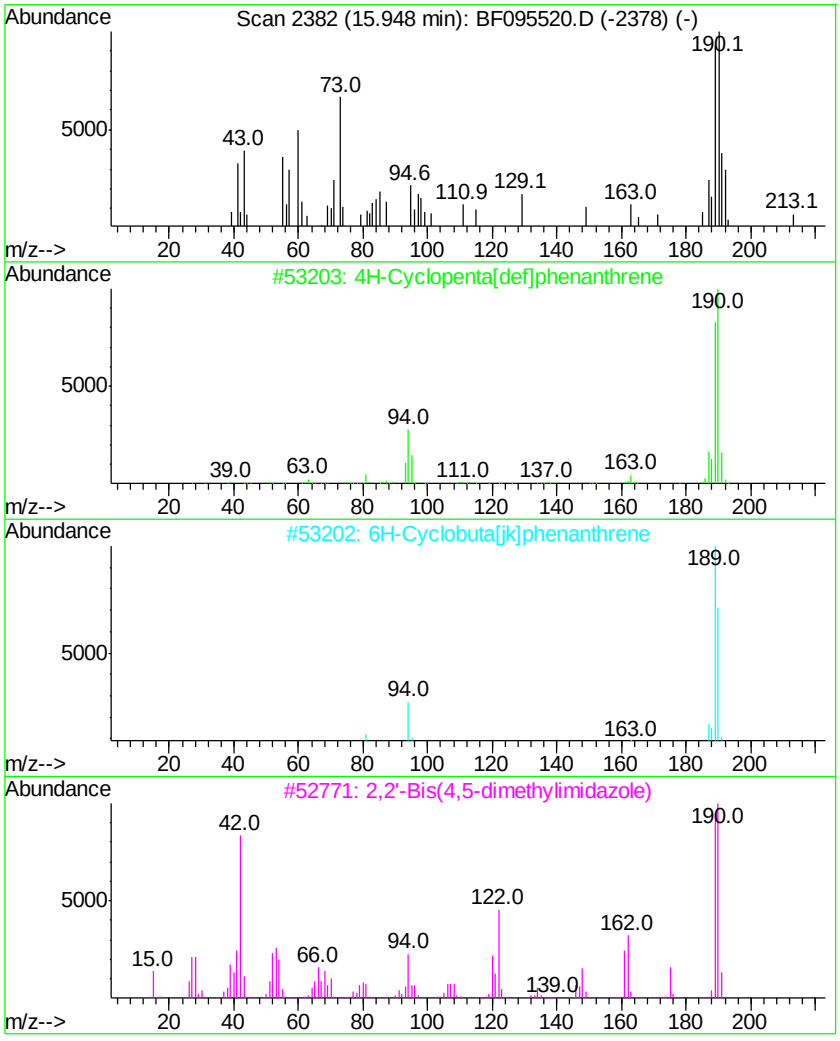
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

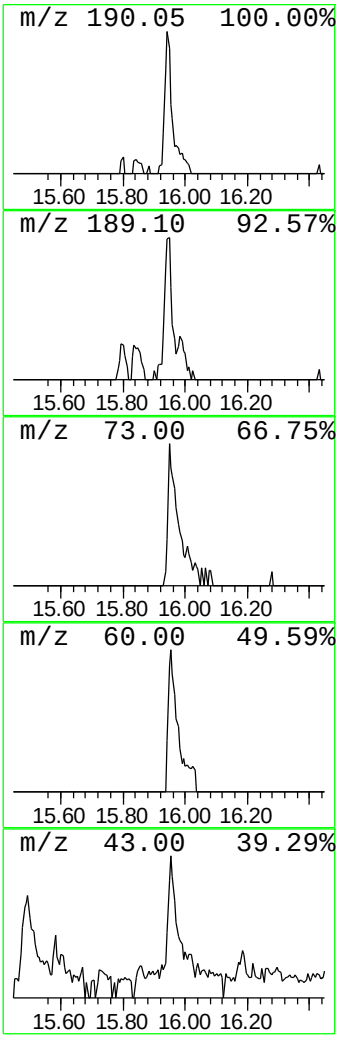
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	4.47 ng	102745	Phenanthrene-d10	15.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	52
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	38
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
4	Isoquinoline, 1-chloro-3-ethyl-	191	C11H10ClN	055150-52-2	22
5	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	17





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Data File : BF095520.D
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Operator : SJ/MA
Sample : I3244-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM8-COMP-0-6

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

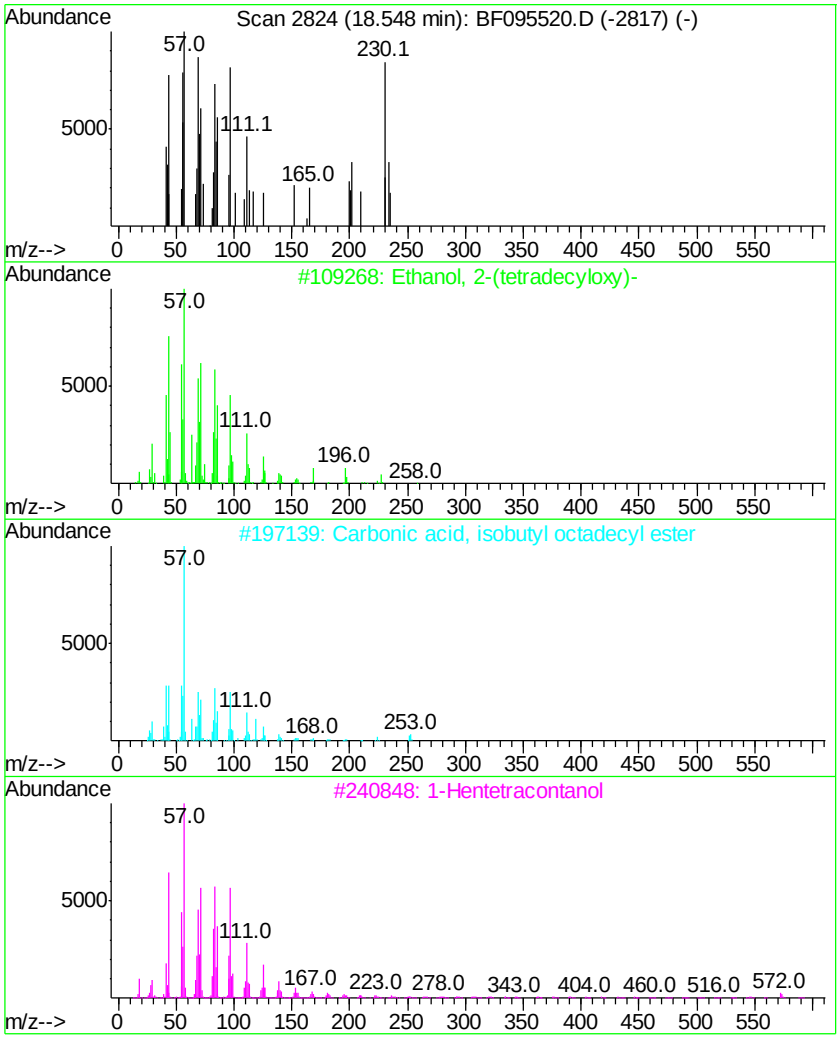
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

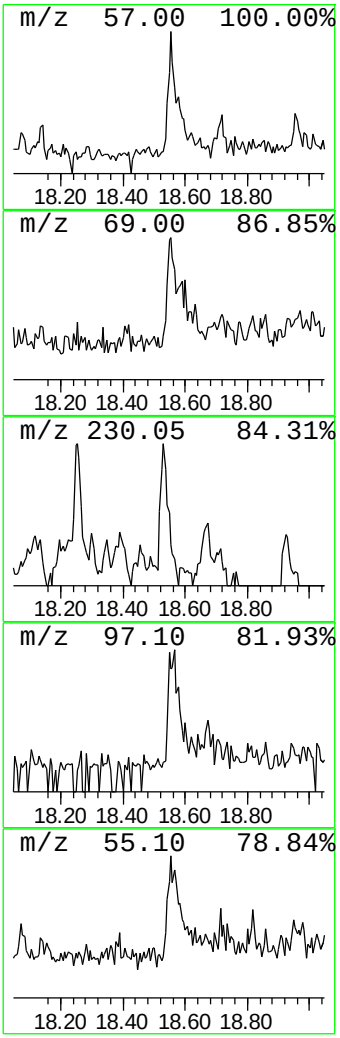
****

Peak Number 6 Ethanol, 2-(tetradecyloxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	2.18 ng	83272	Chrysene-d12	18.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	68
2	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	62
3	1-Hentetracontanol	593	C41H84O	040710-42-7	62
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	58
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	55





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095520.D
Acq On : 28 May 2017 3:42
Operator : SJ/MA
Sample : I3244-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM8-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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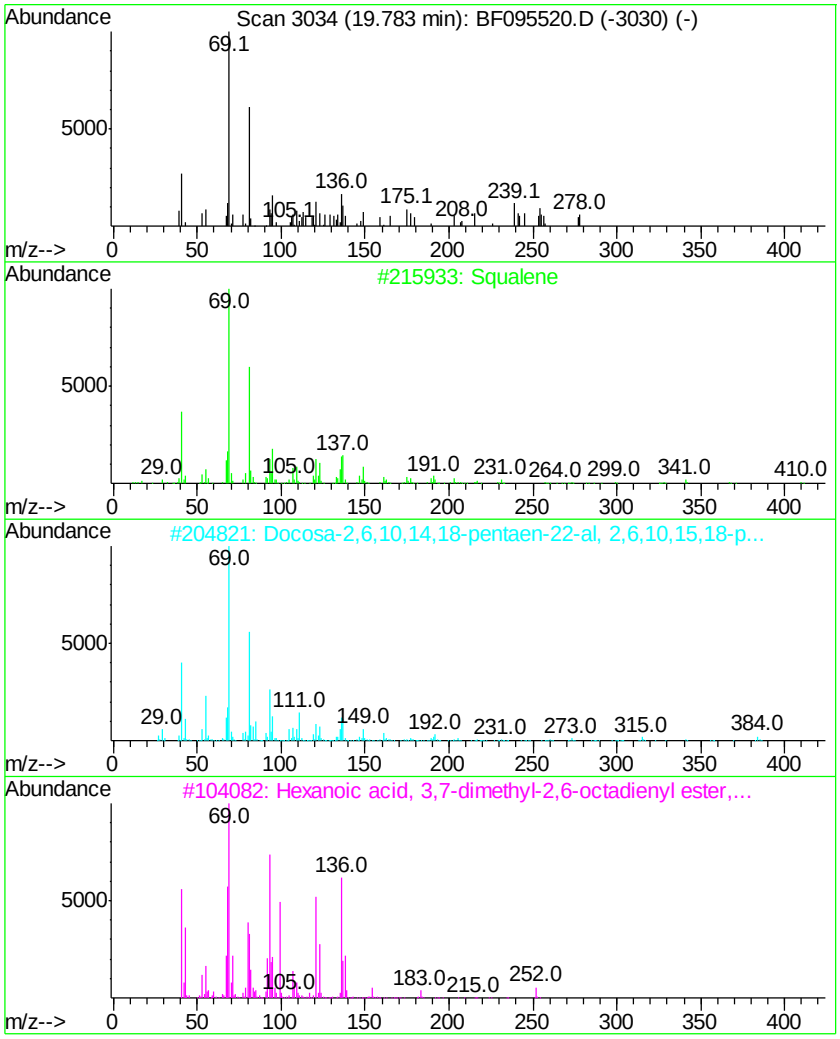
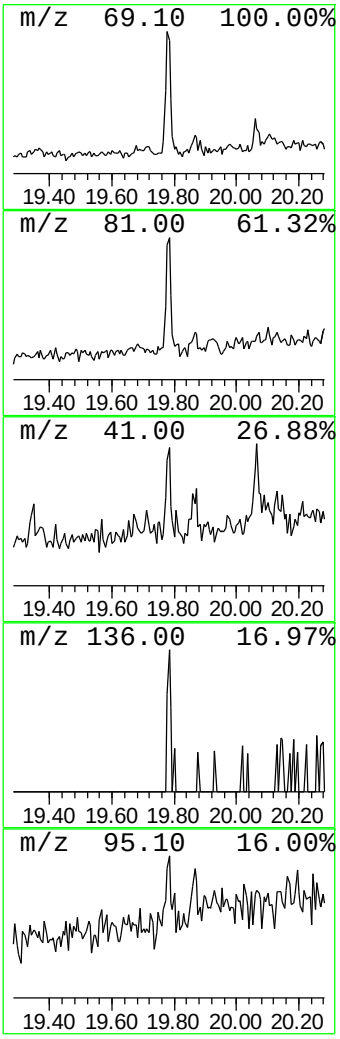
Peak Number 7 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.78	2.31 ng	53638	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	64
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	59
3	Hexanoic acid, 3,7-dimethyl-2,6-...	252	C16H28O2	010032-02-7	59
4	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	58
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	53





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Operator : SJ/MA
Sample : I3244-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM8-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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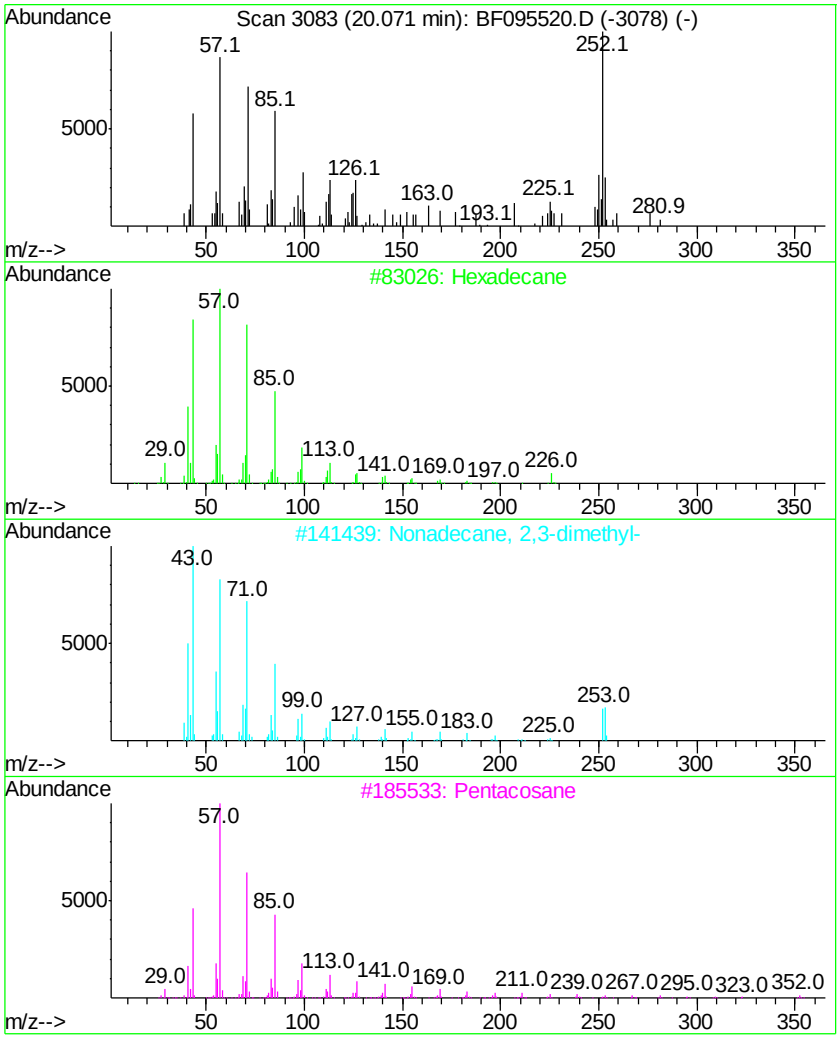
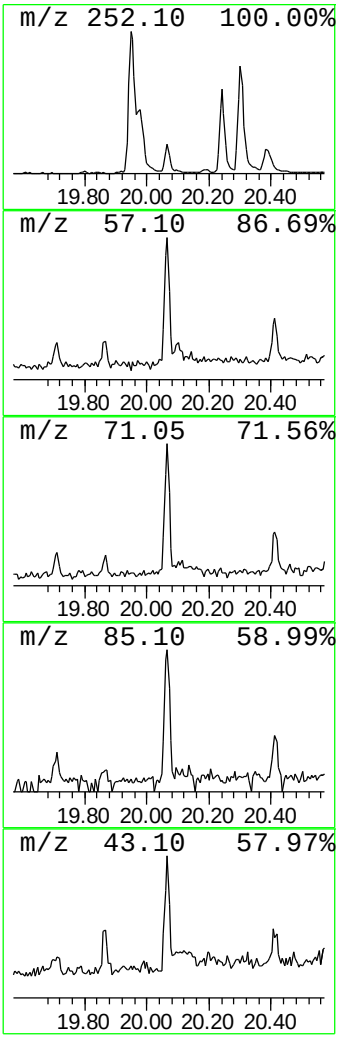
Peak Number 8 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.07	3.37 ng	78463	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	51
2	Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	38
3	Pentacosane	352	C25H52	000629-99-2	38
4	Perylene	252	C20H12	000198-55-0	38
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
Data File : BF095520.D
Acq On : 28 May 2017 3:42
Operator : SJ/MA
Sample : I3244-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM8-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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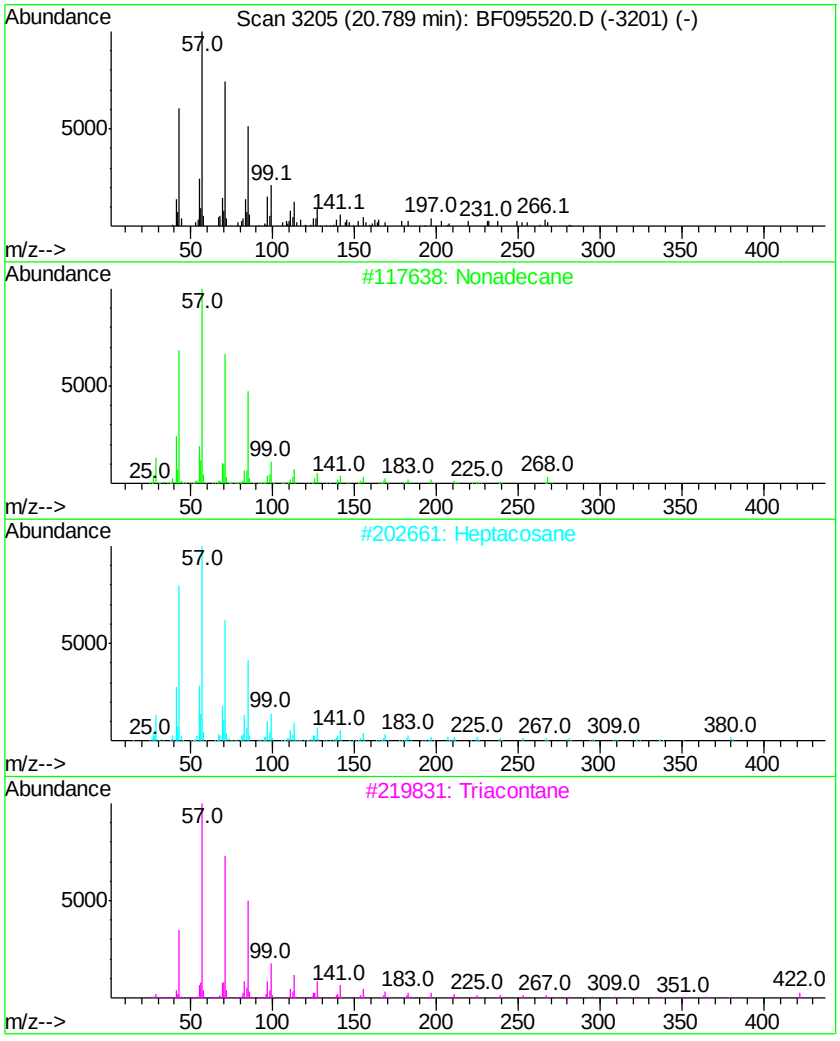
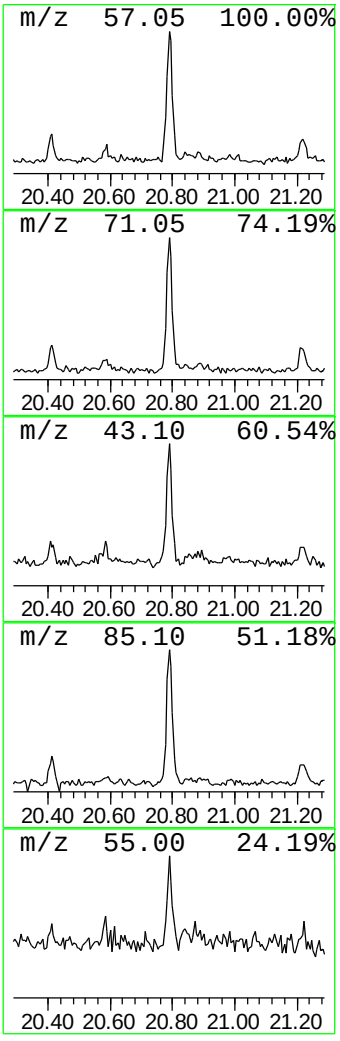
Peak Number 10 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.79	4.20 ng	97806	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Heptacosane	380	C27H56	000593-49-7	90
3	Triacontane	422	C30H62	000638-68-6	90
4	Pentacosane	352	C25H52	000629-99-2	90
5	Heneicosane	296	C21H44	000629-94-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052717\
Data File : BF095520.D
Acq On : 28 May 2017 3:42
Operator : SJ/MA
Sample : I3244-09
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM8-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...	5.10	7.3	ng	201070	1	7.74	554722	20.0
unknown7.40	7.40	79.4	ng	2202580	1	7.74	554722	20.0
1-Tetradecanol	15.49	2.6	ng	59480	4	15.00	459967	20.0
4H-Cyclopenta[def...	15.95	4.5	ng	102745	4	15.00	459967	20.0
Ethanol, 2-(tetra...	18.55	2.2	ng	83272	5	18.67	765542	20.0
Squalene	19.78	2.3	ng	53638	6	20.35	465275	20.0
Hexadecane	20.07	3.4	ng	78463	6	20.35	465275	20.0
Nonadecane	20.79	4.2	ng	97806	6	20.35	465275	20.0