LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095551.D
Acq On : 30 May 2017 23:37
Operator : SJ/MA
Sample : I3302-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-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	5.090	533	536	557	rBV	52115	143021	7.60%	0.926%
2	5.713	638	642	672	rBV	503175	1524349	80.97%	9.873%
3	7.295	907	911	926	rBV	478547	1290723	68.56%	8.360%
4	7.407	926	930	949	rVB	985017	1882656	100.00%	12.194%
5	7.737	982	986	995	rBV	389138	496574	26.38%	3.216%
6	7.972	1021	1026	1042	rBV	988614	1273987	67.67%	8.252%
7	8.648	1137	1141	1166	rBV	343576	855262	45.43%	5.540%
8	9.766	1326	1331	1357	rBV	255049	629260	33.42%	4.076%
9	11.536	1627	1632	1653	rBV	746173	1415483	75.19%	9.168%
10	12.242	1748	1752	1770	rBV	67293	155013	8.23%	1.004%
11	12.601	1808	1813	1829	rBV	324472	615932	32.72%	3.989%
12	13.424	1948	1953	1958	rBV	20711	26681	1.42%	0.173%
13	13.901	2030	2034	2057	rBV	305298	671495	35.67%	4.349%
14	14.195	2080	2084	2087	rBV3	17259	23453	1.25%	0.152%
15	15.001	2217	2221	2226	rBV2	255889	408715	21.71%	2.647%
16	15.842	2360	2364	2370	rBV3	11364	19207	1.02%	0.124%
17	15.954	2378	2383	2396	rVB5	67671	139639	7.42%	0.904%
18	16.789	2520	2525	2533	rBV	140936	193958	10.30%	1.256%
19	17.089	2571	2576	2585	rVB	169826	227288	12.07%	1.472%
20	17.312	2610	2614	2625	rBV	771871	953037	50.62%	6.173%
21	17.406	2627	2630	2636	rVB4	11692	22084	1.17%	0.143%
22	17.554	2652	2655	2662	rVB	19408	25819	1.37%	0.167%
23	17.642	2666	2670	2674	rBV2	14398	20593	1.09%	0.133%
24	17.689	2674	2678	2683	rBV3	19676	32553	1.73%	0.211%
25	18.006	2728	2732	2738	rVV2	23848	35246	1.87%	0.228%
26	18.553	2821	2825	2836	rVB4	33230	71031	3.77%	0.460%
27	18.671	2840	2845	2850	rBV2	447457	686756	36.48%	4.448%
28	18.806	2865	2868	2873	rBV3	16786	23683	1.26%	0.153%
29	18.959	2891	2894	2900	rVV6	13231	21305	1.13%	0.138%
30	19.183	2929	2932	2936	rBV3	17510	23323	1.24%	0.151%
31	19.342	2955	2959	2961	rBV3	35075	38336	2.04%	0.248%
32	19.712	3019	3022	3026	rVB4	23979	25895	1.38%	0.168%
33	19.783	3030	3034	3038	rBV	43807	57099	3.03%	0.370%
34	19.865	3045	3048	3053	rVB6	23523	28933	1.54%	0.187%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
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Acq On : 30 May 2017 23:37
Operator : SJ/MA
Sample : I3302-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-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	19.953	3058	3063	3066	rBV	75710	123331	6.55%	0.799%
36	20.065	3078	3082	3085	rBV	93710	106407	5.65%	0.689%
37	20.242	3109	3112	3116	rVB	33275	37525	1.99%	0.243%
38	20.300	3119	3122	3126	rVV	53015	63954	3.40%	0.414%
39	20.353	3127	3131	3138	rVV	260509	381420	20.26%	2.470%
40	20.412	3138	3141	3146	rVB2	46949	61976	3.29%	0.401%
41	20.583	3167	3170	3174	rVB4	41161	47089	2.50%	0.305%
42	20.789	3201	3205	3210	rBV2	111077	147558	7.84%	0.956%
43	20.842	3212	3214	3218	rVV5	19519	24446	1.30%	0.158%
44	21.218	3274	3278	3284	rBV2	41481	57971	3.08%	0.375%
45	21.724	3358	3364	3370	rVB5	115649	230154	12.22%	1.491%
46	22.112	3424	3430	3433	rBV8	24285	60016	3.19%	0.389%
47	22.283	3457	3459	3466	rVB4	22740	38899	2.07%	0.252%

Sum of corrected areas: 15439135

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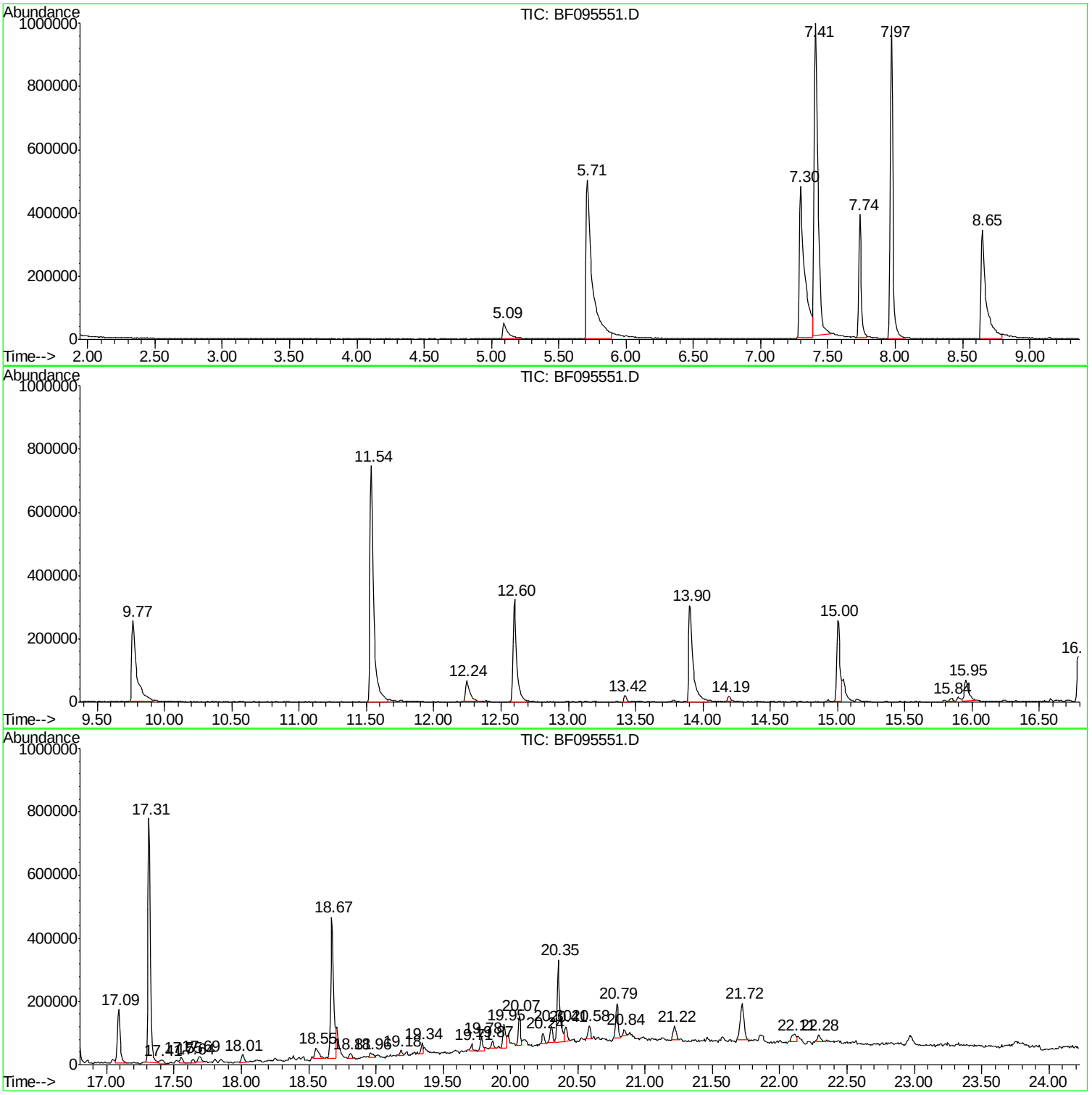
BNA_F
ClientSampleId :
NM15-COMP-0-6

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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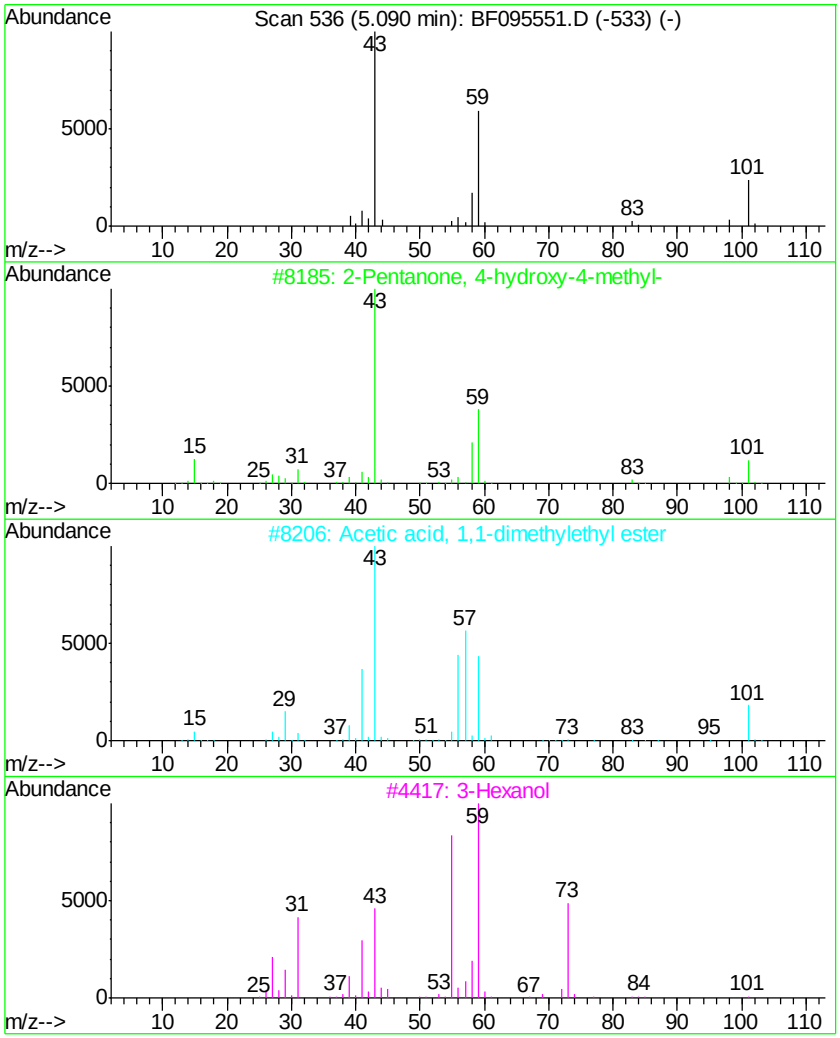
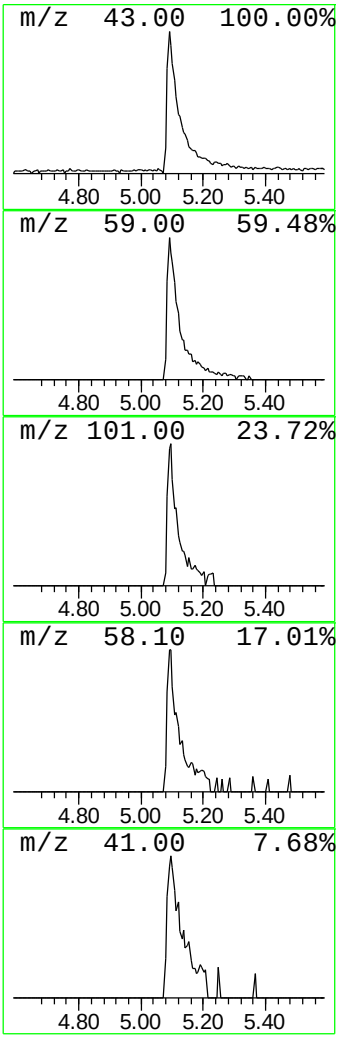
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	5.76 ng	143021	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	53
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	40
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	9





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Instrument : BNA_F
ClientSampleId : NM15-COMP-0-6

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

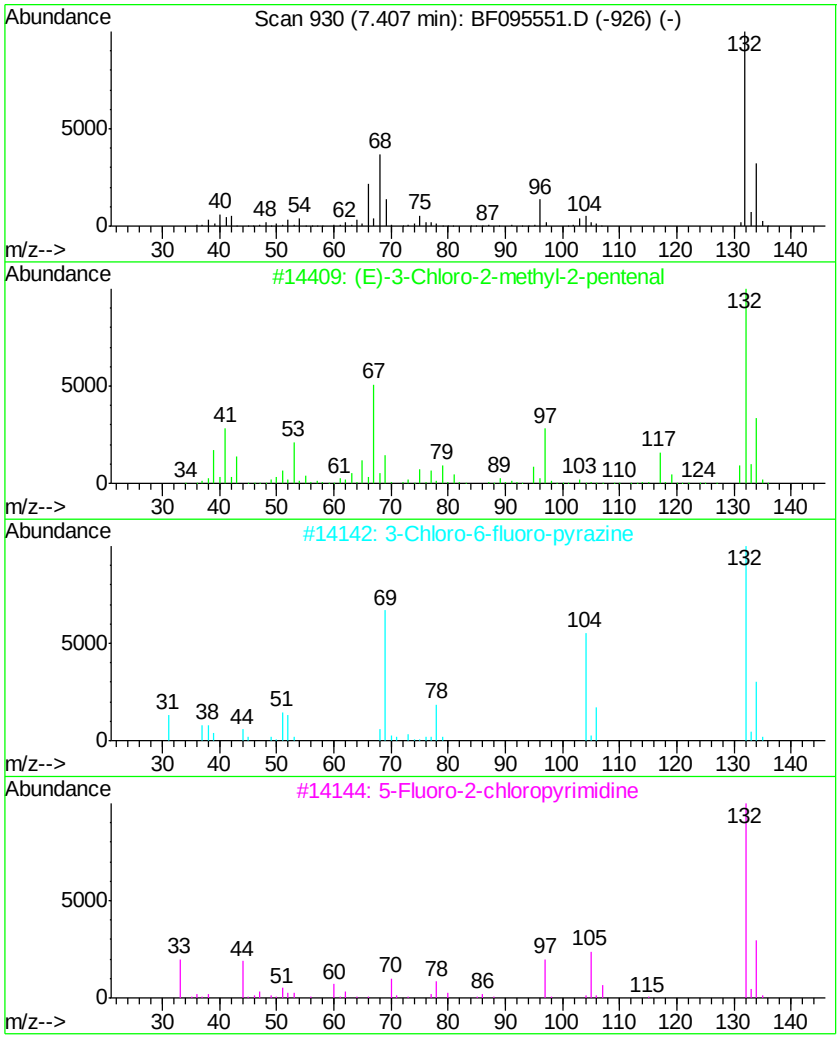
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

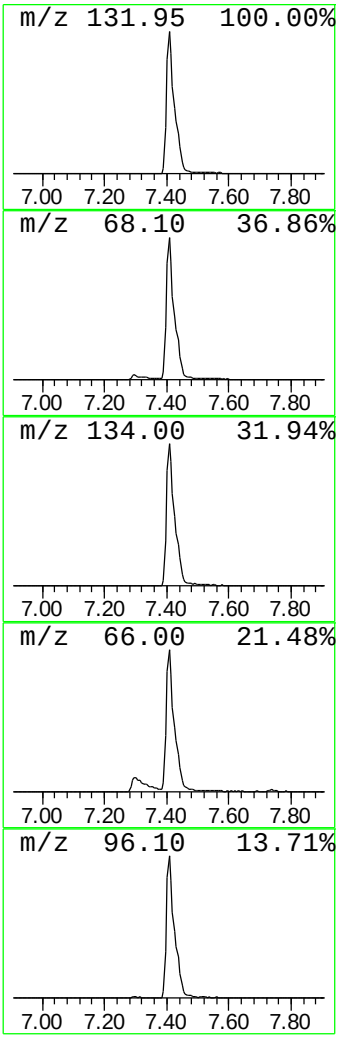
****

Peak Number 2 unknown7.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	75.83 ng	1882660	1,4-Dichlorobenzene-d4	7.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Sample : I3302-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-COMP-0-6

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

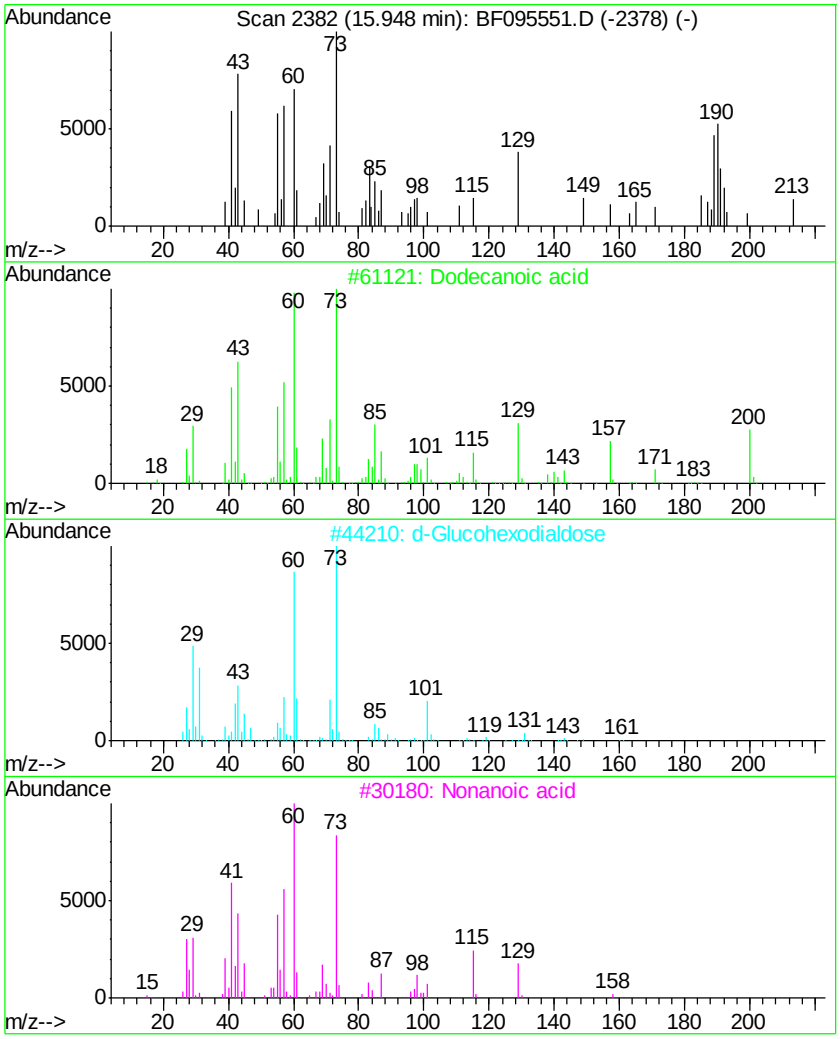
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

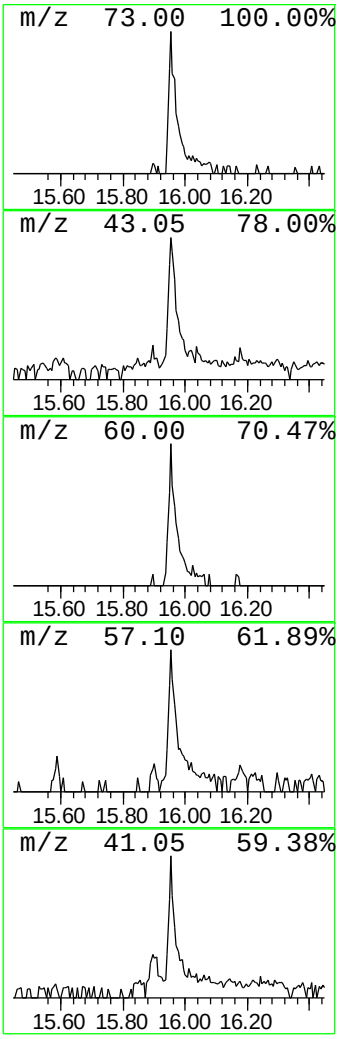
****

Peak Number 4 unknown15.95 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	6.83 ng	139639	Phenanthrene-d10	15.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	47
2	d-Glucohexodialdose	178	C6H10O6	1000149-19-1	38
3	Nonanoic acid	158	C9H18O2	000112-05-0	27
4	Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	18
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	15





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Sample : I3302-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-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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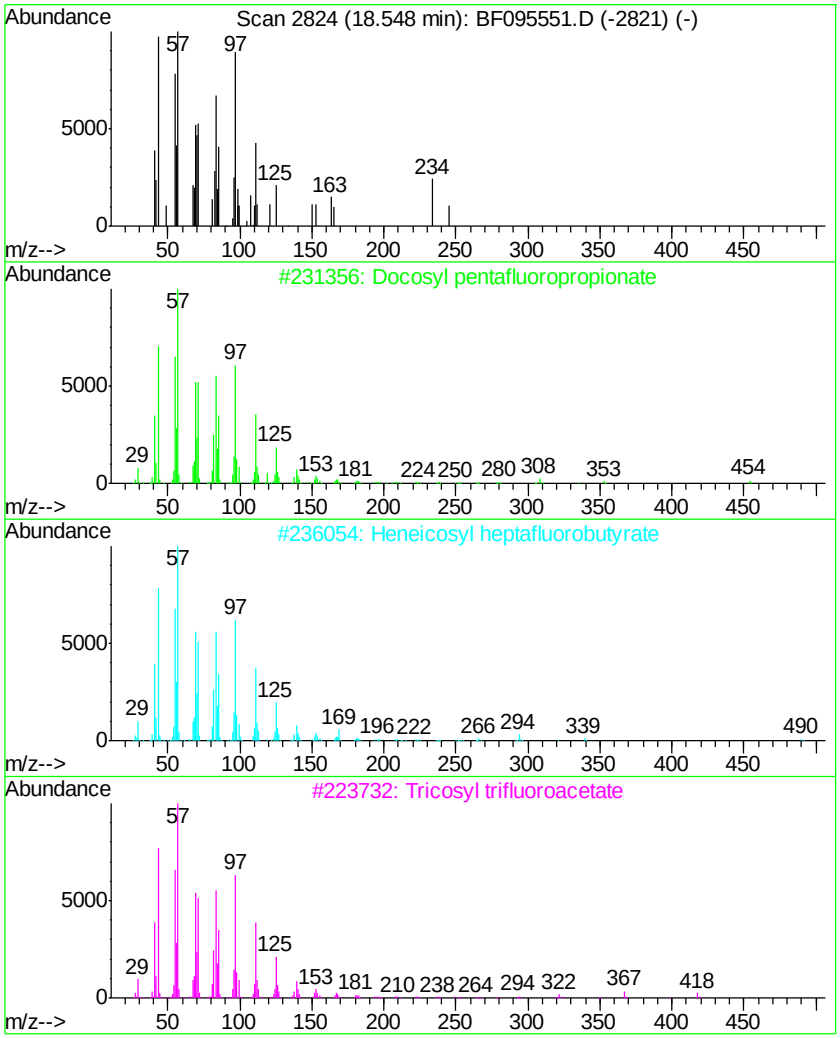
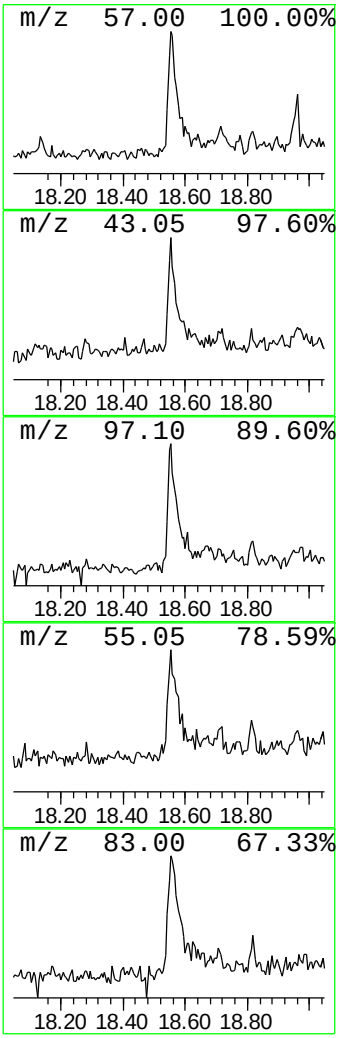
Peak Number 5 Docosyl pentafluoropropionate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	2.07 ng	71031	Chrysene-d12	18.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
2	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	90
4	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	90
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87





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Sample : I3302-09
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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-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
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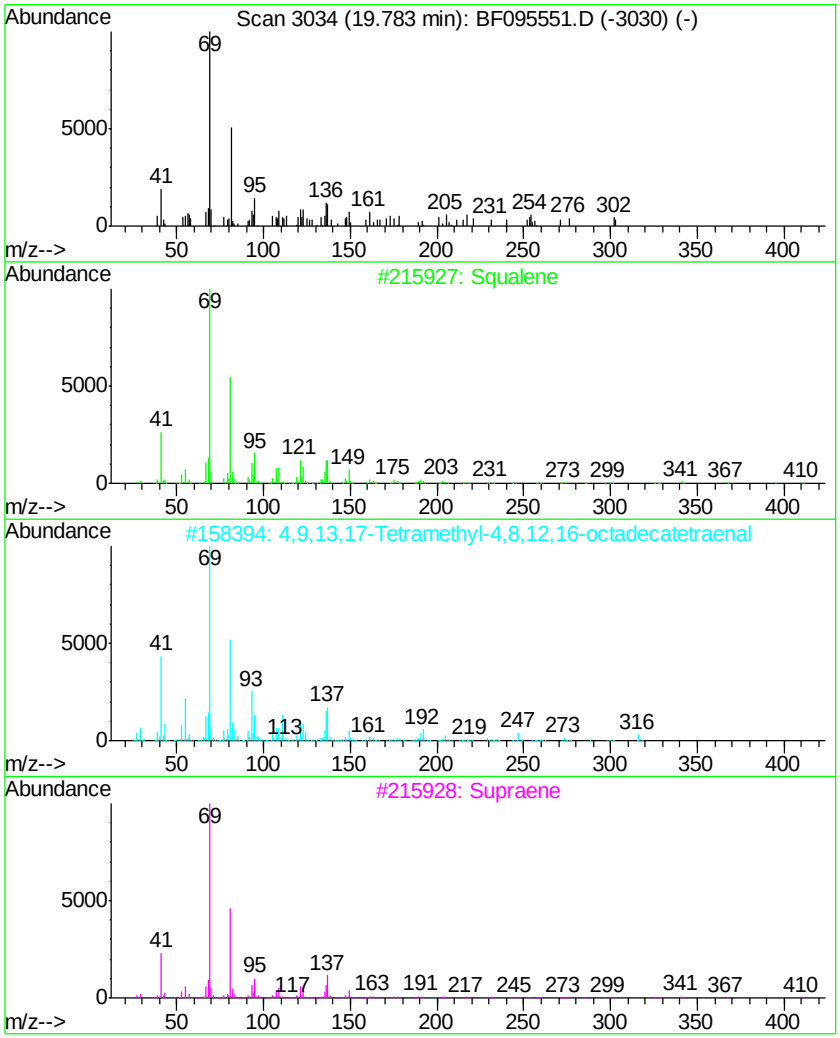
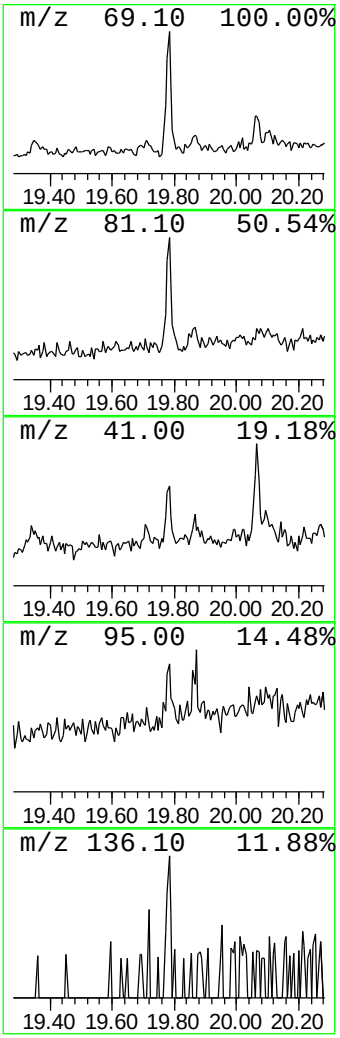
Peak Number 6 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.78	2.99 ng	57099	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	64
2	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	59
3	Supraene	410	C30H50	007683-64-9	59
4	Furan, 3-(4,8-dimethyl-3,7-nonad...	218	C15H22O	023262-34-2	59
5	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	59





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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-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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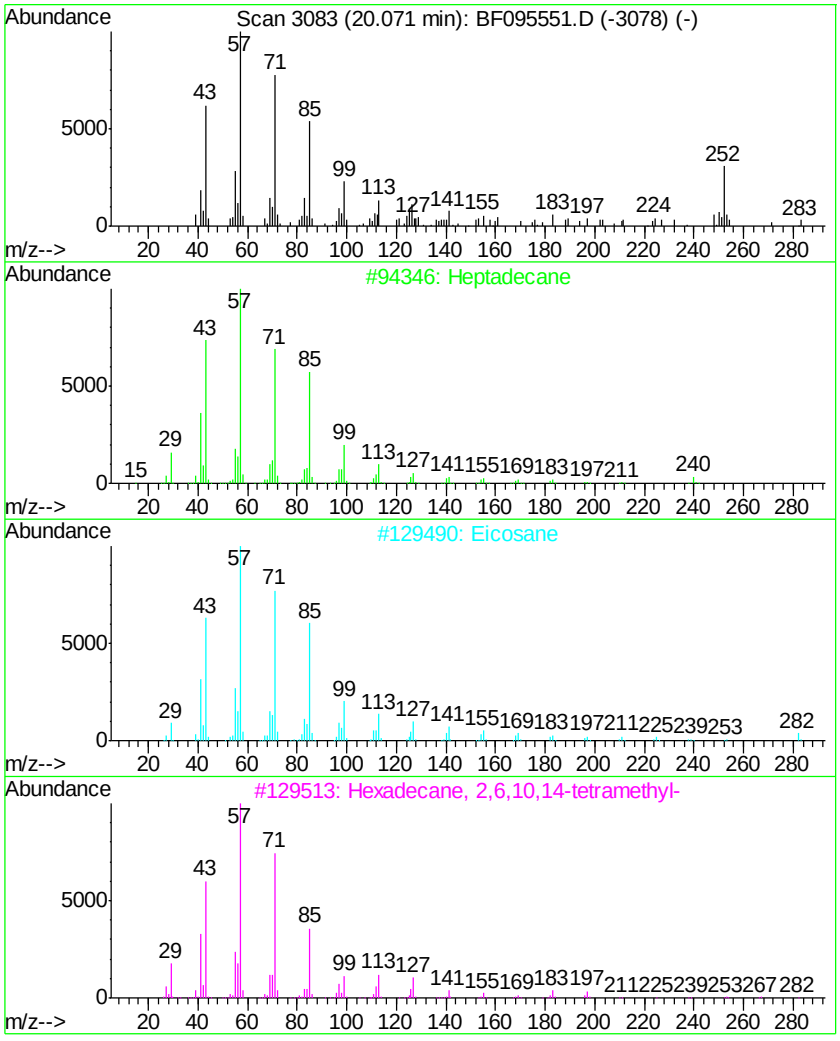
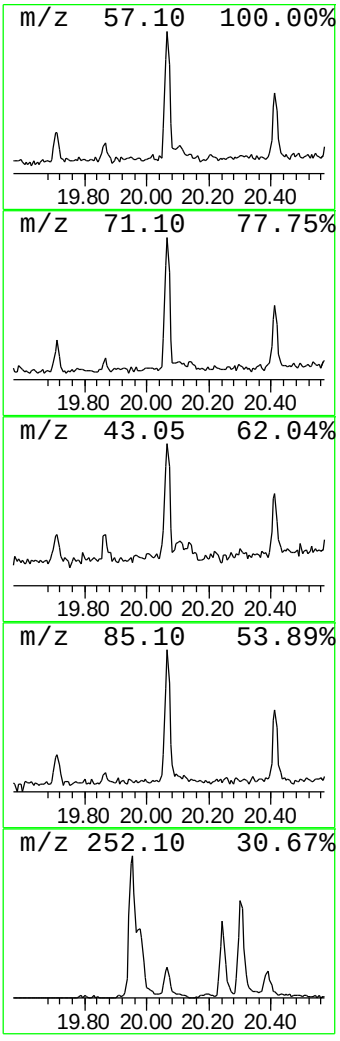
Peak Number 7 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.07	5.58 ng	106407	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Eicosane	282	C20H42	000112-95-8	89
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	76
4	Heneicosane	296	C21H44	000629-94-7	76
5	Hexacosane	366	C26H54	000630-01-3	64





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Instrument : BNA_F
ClientSampleId : NM15-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

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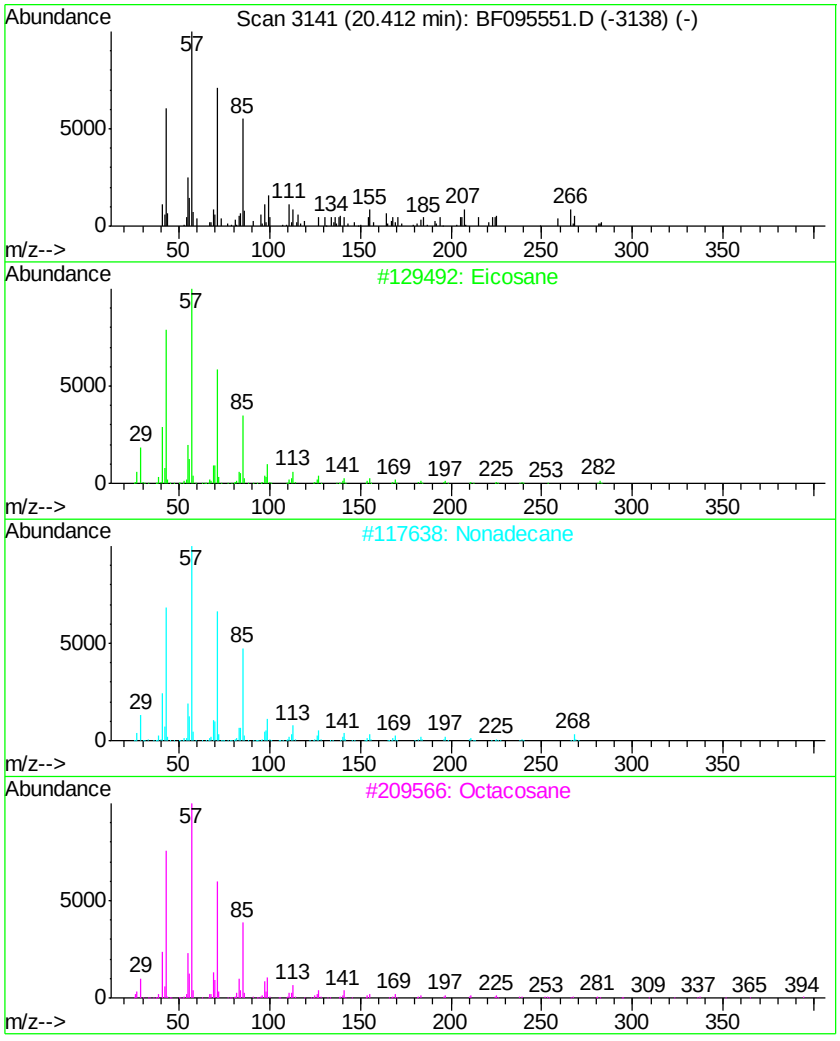
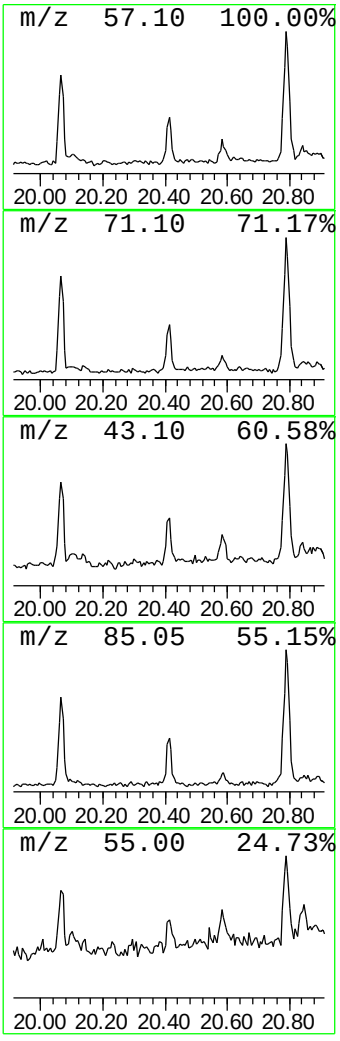
Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.41	3.25 ng	61976	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	68
2	Nonadecane	268	C19H40	000629-92-5	64
3	Octacosane	394	C28H58	000630-02-4	59
4	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	59
5	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	59





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Data File : BF095551.D
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Operator : SJ/MA
Sample : I3302-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-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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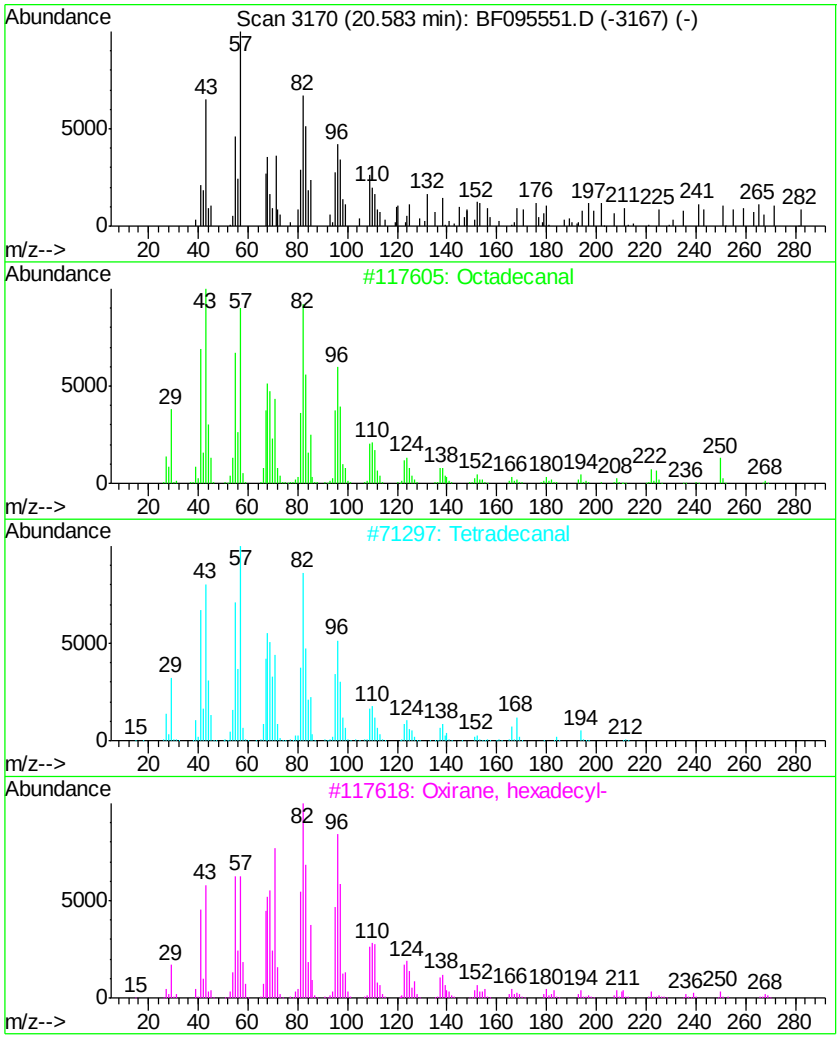
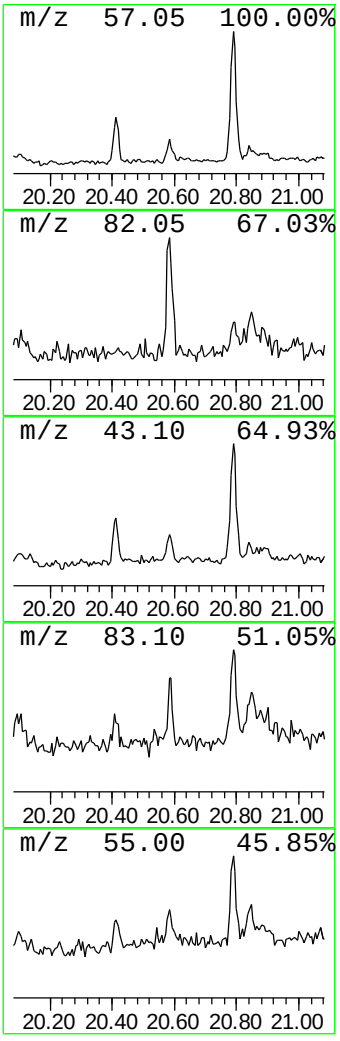
Peak Number 9 Octadecanal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.58	2.47 ng	47089	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	58
2	Tetradecanal	212	C14H28O	000124-25-4	50
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	49
4	12-Octadecenal	266	C18H34O	056554-91-7	45
5	13-Octadecenal	266	C18H34O	056554-90-6	43





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Instrument : BNA_F
ClientSampleId : NM15-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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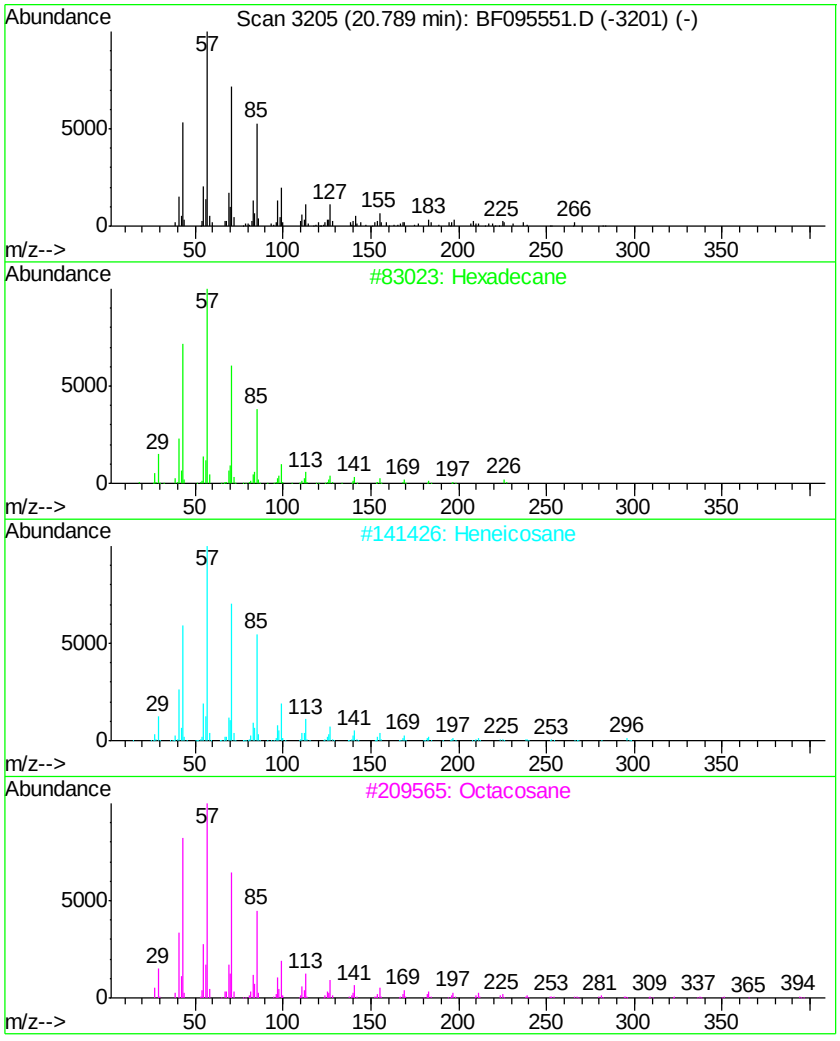
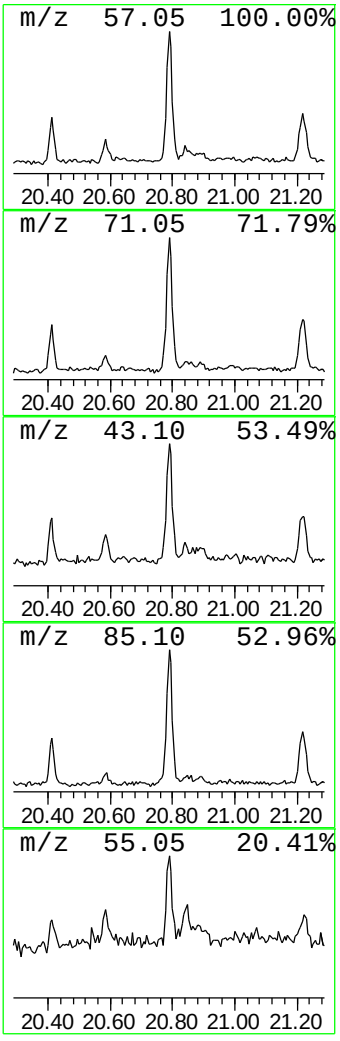
Peak Number 10 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.79	7.74 ng	147558	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heptacosane	380	C27H56	000593-49-7	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095551.D
Acq On : 30 May 2017 23:37
Operator : SJ/MA
Sample : I3302-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-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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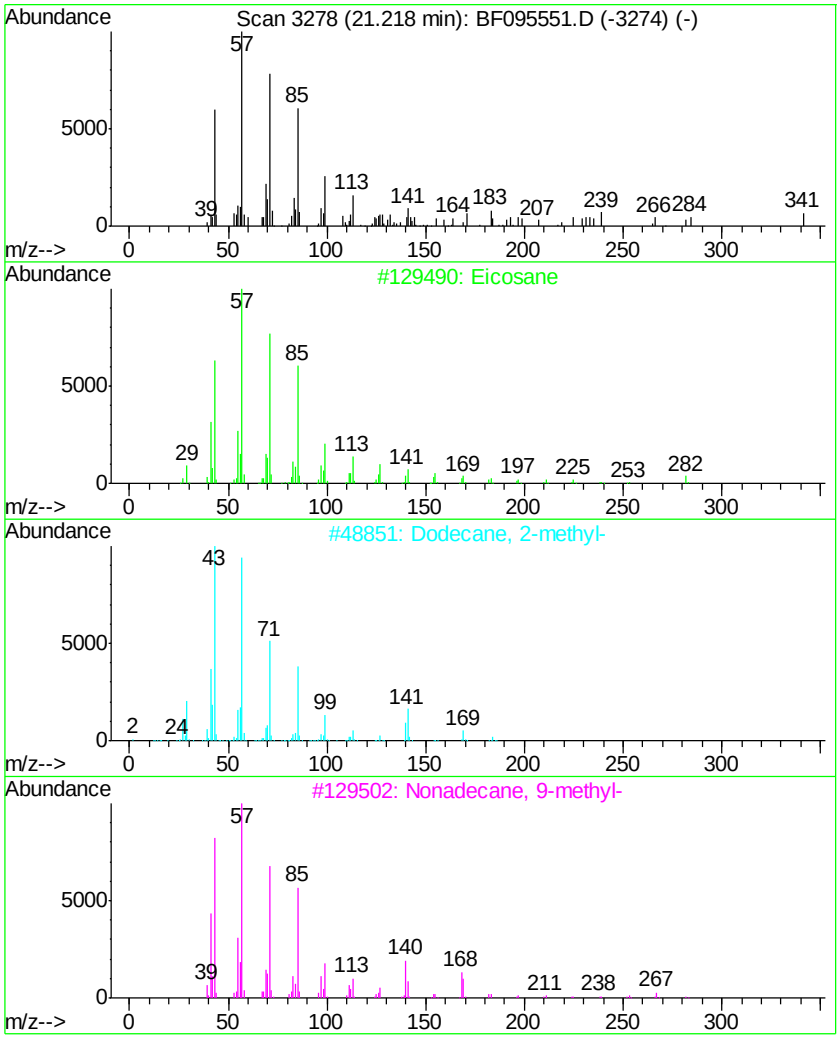
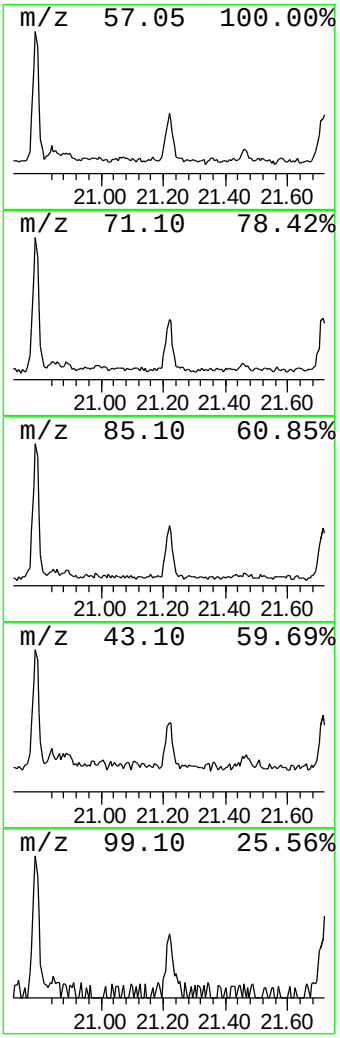
Peak Number 11 Dodecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.22	3.04 ng	57971	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	89
2	Dodecane, 2-methyl-	184	C13H28	001560-97-0	72
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	72
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72
5	Heptadecane	240	C17H36	000629-78-7	72





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Acq On : 30 May 2017 23:37
Operator : SJ/MA
Sample : I3302-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-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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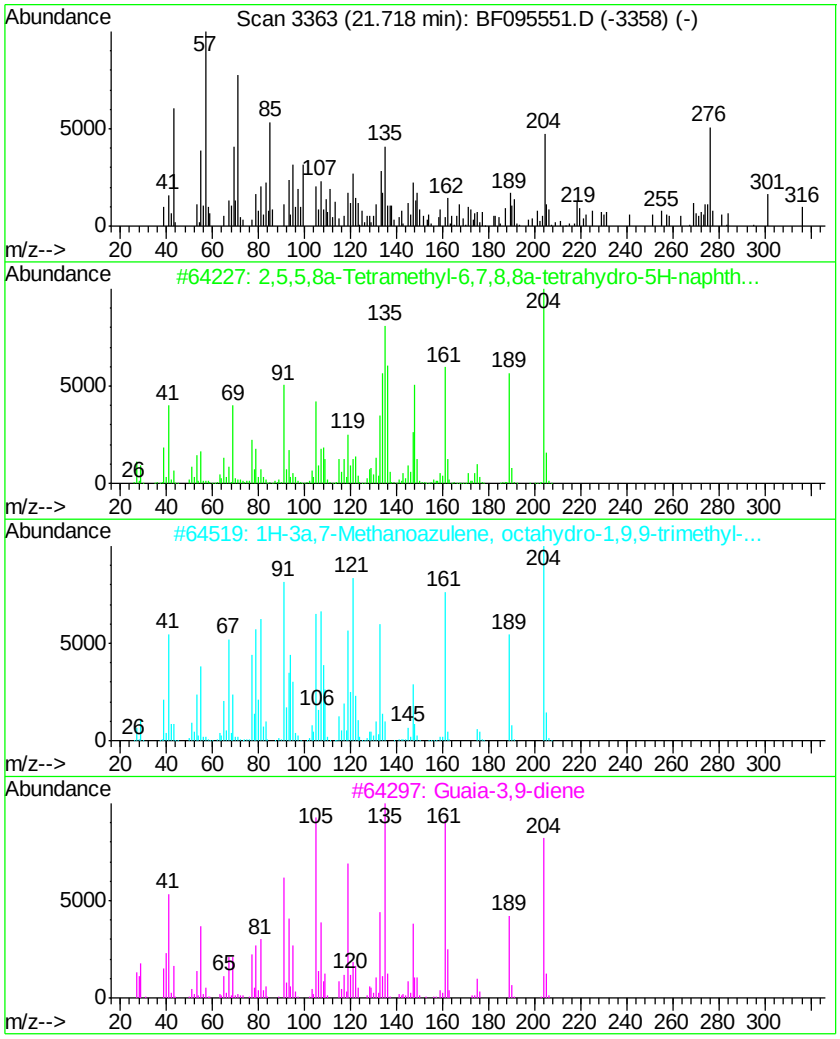
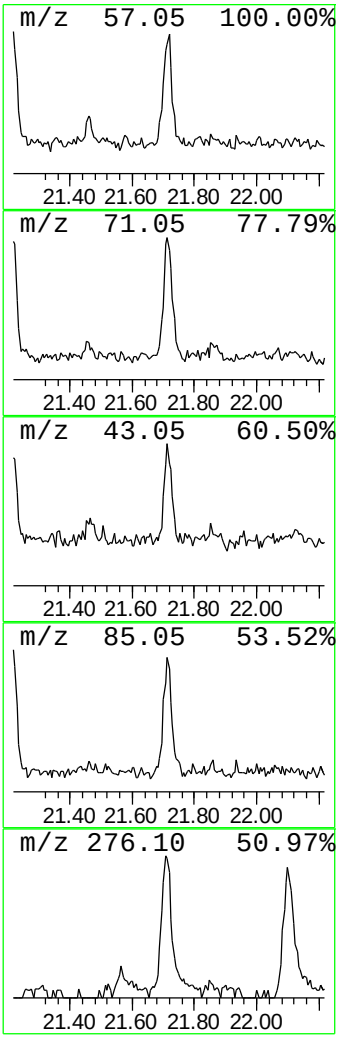
Peak Number 12 2,5,5,8a-Tetramethyl-6,7,8,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.72	12.07 ng	230154	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	60
2	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	46
3	Guaia-3,9-diene	204	C15H24	000489-83-8	46
4	5-Azulenemethanol, 1,2,3,4,5,6,7...	264	C17H28O2	000134-28-1	46
5	1,4-Methanoazulen-9-ol, decahydr...	222	C15H26O	000465-24-7	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095551.D
Acq On : 30 May 2017 23:37
Operator : SJ/MA
Sample : I3302-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
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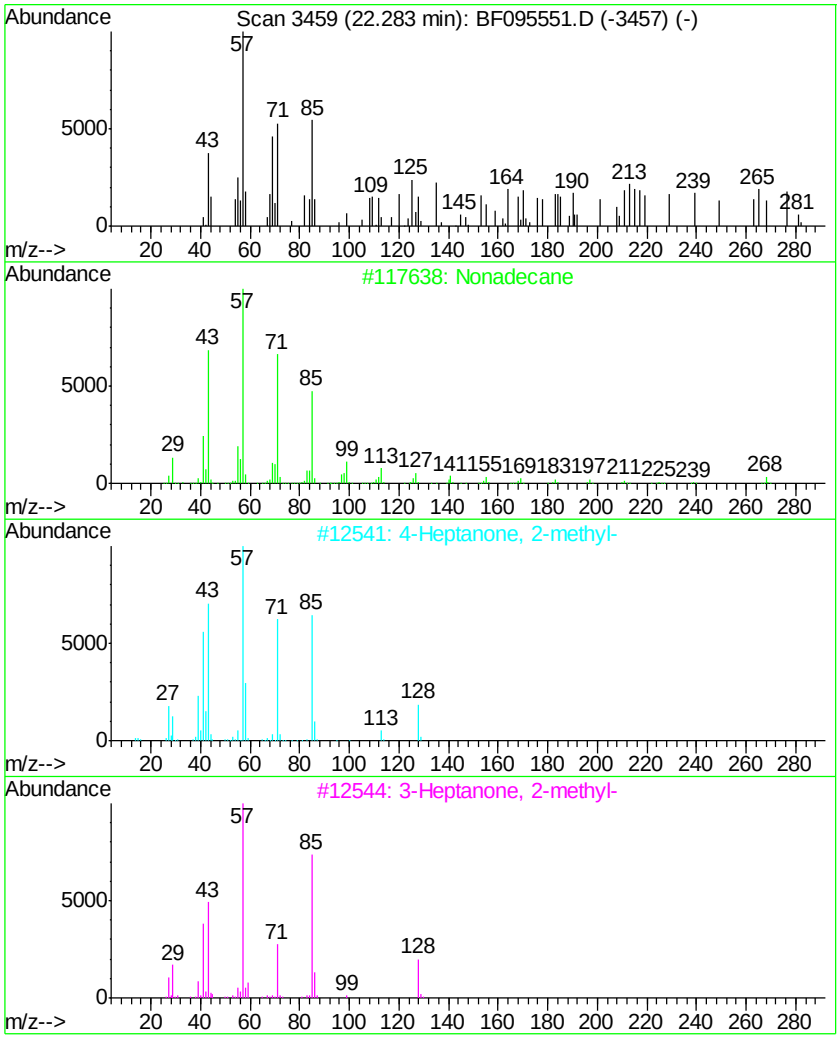
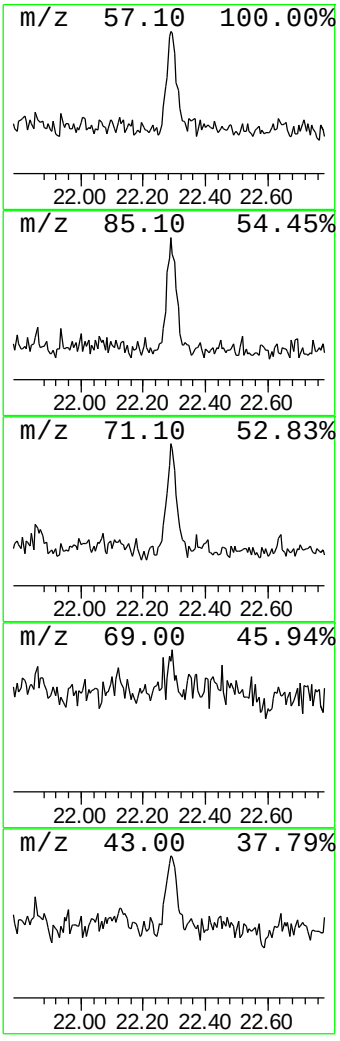
Peak Number 13 unknown22.28 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	2.04 ng	38899	Perylene-d12	20.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	14
2	4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	11
3	3-Heptanone, 2-methyl-	128	C8H16O	013019-20-0	11
4	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	11
5	Phendimetrazine	191	C12H17NO	000634-03-7	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095551.D
Acq On : 30 May 2017 23:37
Operator : SJ/MA
Sample : I3302-09
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-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...	5.09	5.8	ng	143021	1	7.74	496574	20.0
unknown7.41	7.41	75.8	ng	1882660	1	7.74	496574	20.0
unknown15.95	15.95	6.8	ng	139639	4	15.01	408715	20.0
Docosyl pentafluo...	18.55	2.1	ng	71031	5	18.67	686756	20.0
Squalene	19.78	3.0	ng	57099	6	20.35	381420	20.0
Heptadecane	20.07	5.6	ng	106407	6	20.35	381420	20.0
Eicosane	20.41	3.3	ng	61976	6	20.35	381420	20.0
Octadecanal	20.58	2.5	ng	47089	6	20.35	381420	20.0
Hexadecane	20.79	7.7	ng	147558	6	20.35	381420	20.0
Dodecane, 2-methyl-	21.22	3.0	ng	57971	6	20.35	381420	20.0
2,5,5,8a-Tetramet...	21.72	12.1	ng	230154	6	20.35	381420	20.0
unknown22.28	22.28	2.0	ng	38899	6	20.35	381420	20.0