

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
 Data File : BF095283.D
 Acq On : 20 May 2017 1:55
 Operator : SJ/MA
 Sample : I3202-03
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3COMP

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	564	rBV	187526	516092	19.50%	2.635%
2	5.731	641	645	677	rBV	813278	1918910	72.51%	9.799%
3	7.301	908	912	929	rBV	1137778	1947504	73.59%	9.945%
4	7.425	929	933	949	rVB	1501379	2325870	87.89%	11.877%
5	7.760	987	990	1001	rBV	428732	543345	20.53%	2.775%
6	8.001	1026	1031	1047	rBV	1189868	1523408	57.57%	7.779%
7	8.660	1139	1143	1171	rBV	762194	1261122	47.66%	6.440%
8	9.783	1329	1334	1354	rBV	380019	643428	24.31%	3.286%
9	11.548	1629	1634	1667	rBV	1794740	2646247	100.00%	13.513%
10	12.254	1749	1754	1766	rBV	160811	260578	9.85%	1.331%
11	12.613	1810	1815	1828	rBV2	525250	814688	30.79%	4.160%
12	13.448	1953	1957	1963	rBV	30462	35179	1.33%	0.180%
13	13.907	2030	2035	2054	rBV	702569	1196401	45.21%	6.110%
14	14.218	2083	2088	2091	rBV	34300	41239	1.56%	0.211%
15	15.018	2219	2224	2241	rVV	398713	616409	23.29%	3.148%
16	15.759	2346	2350	2357	rBV	111301	128876	4.87%	0.658%
17	15.971	2380	2386	2396	rBV4	36136	77178	2.92%	0.394%
18	16.718	2508	2513	2515	rBV	221162	218294	8.25%	1.115%
19	16.748	2515	2518	2522	rVV	321127	335429	12.68%	1.713%
20	16.877	2535	2540	2544	rBV	54967	56928	2.15%	0.291%
21	17.336	2613	2618	2629	rBV	1210337	1469260	55.52%	7.503%
22	18.583	2824	2830	2838	rBV6	25616	76909	2.91%	0.393%
23	18.689	2844	2848	2862	rBV	317241	458982	17.34%	2.344%
24	20.365	3129	3133	3142	rBV	308393	470136	17.77%	2.401%

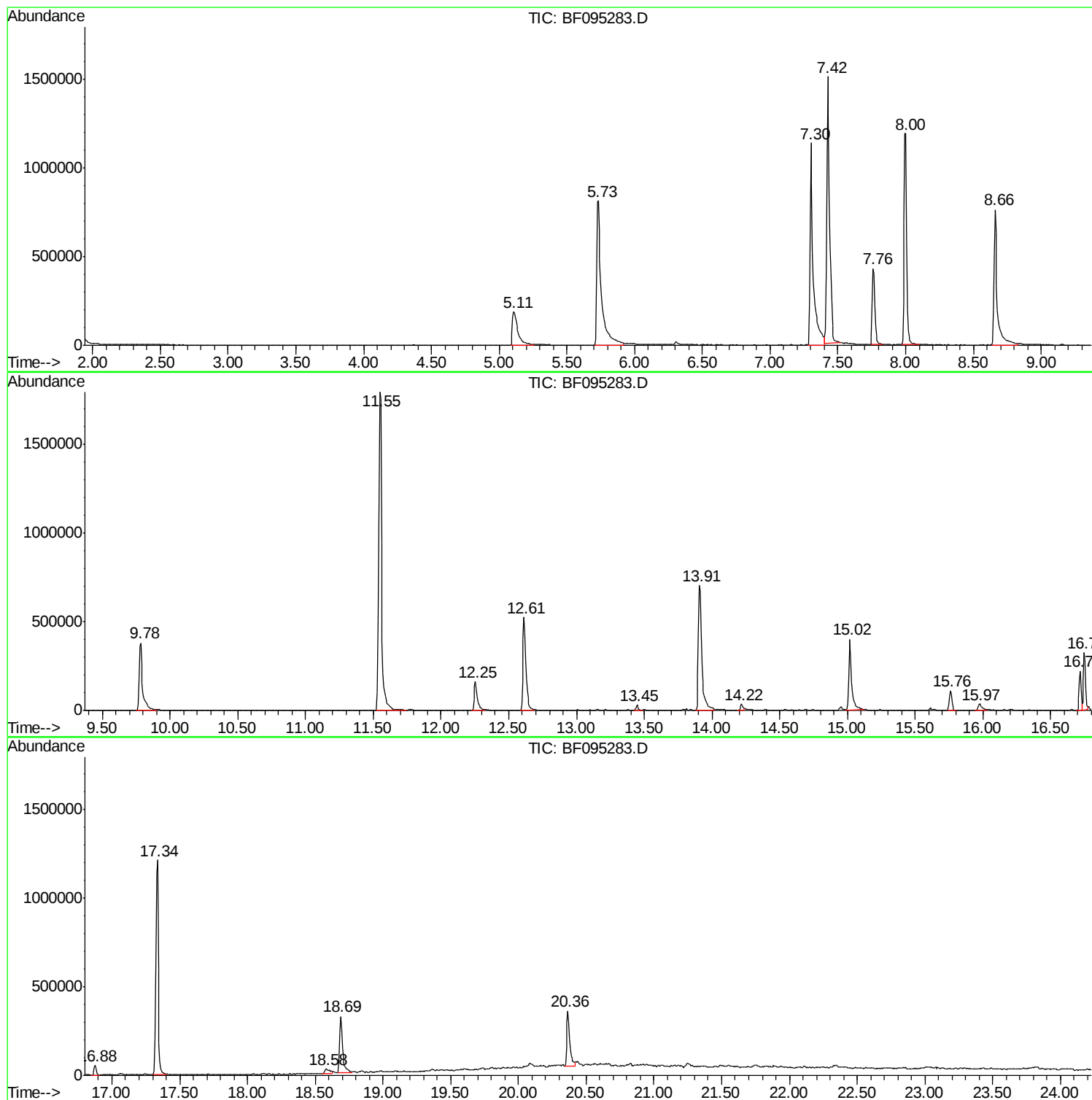
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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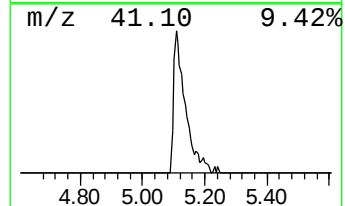
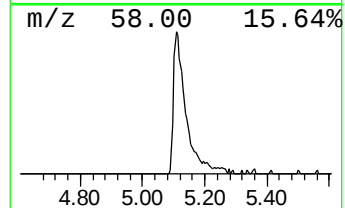
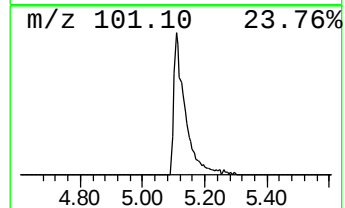
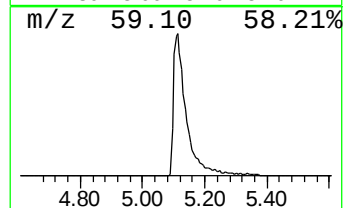
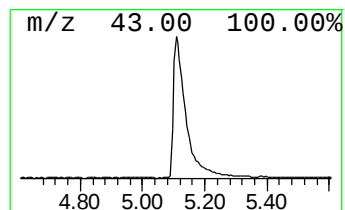
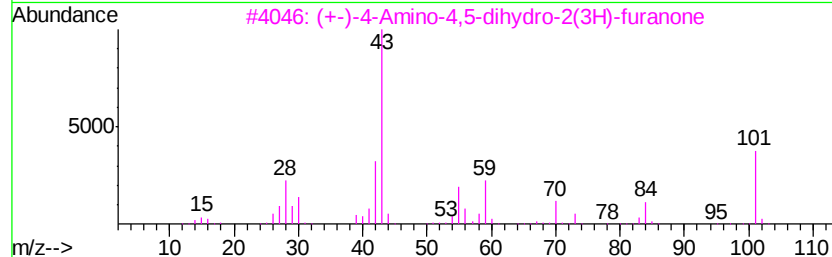
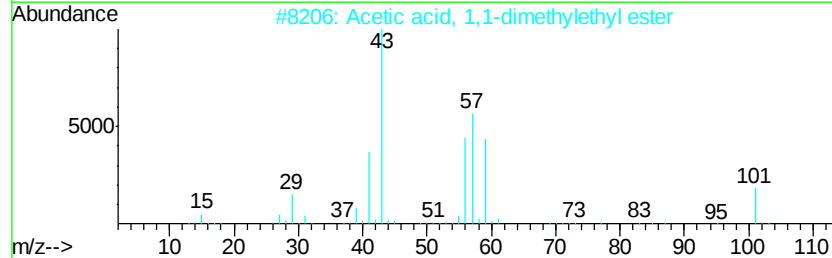
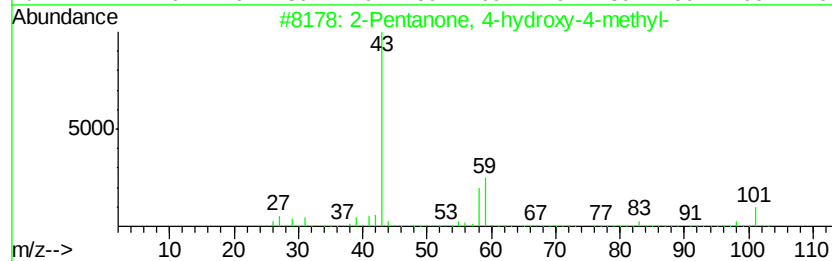
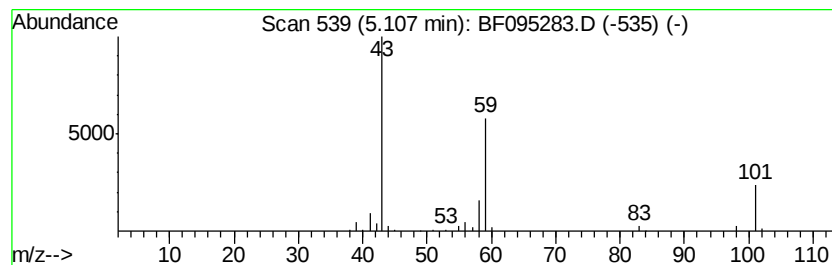
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	19.00 ng	516092	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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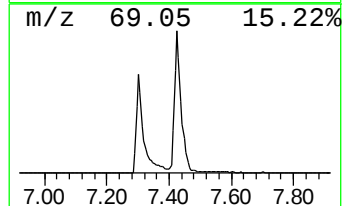
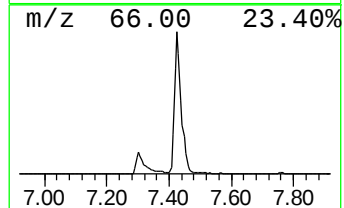
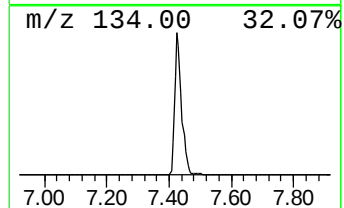
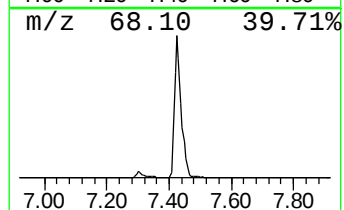
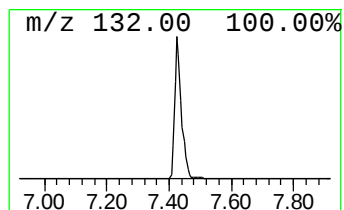
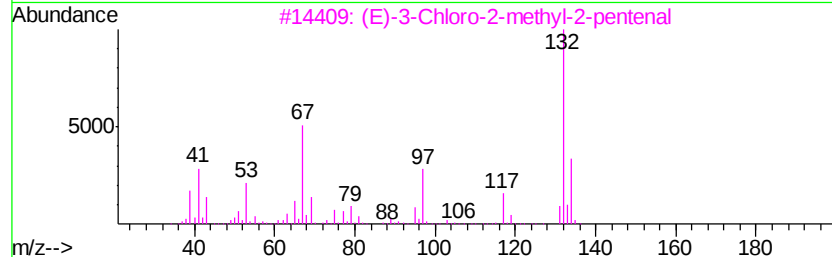
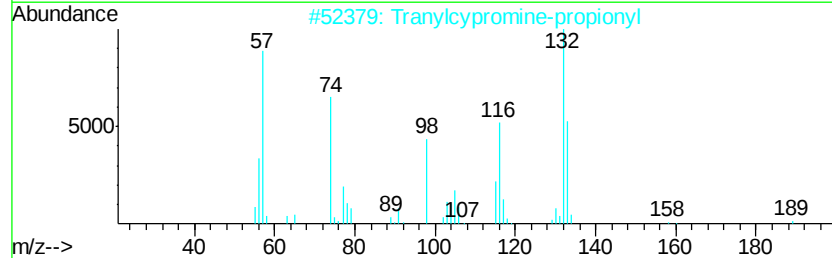
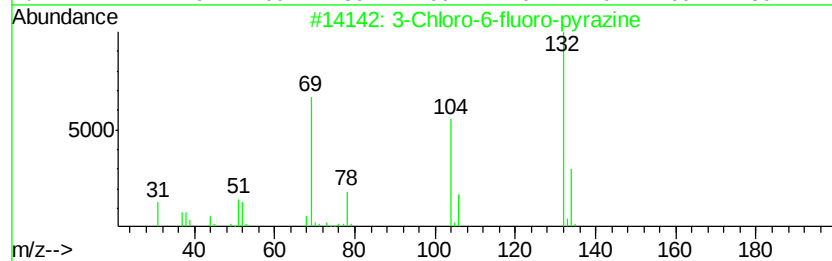
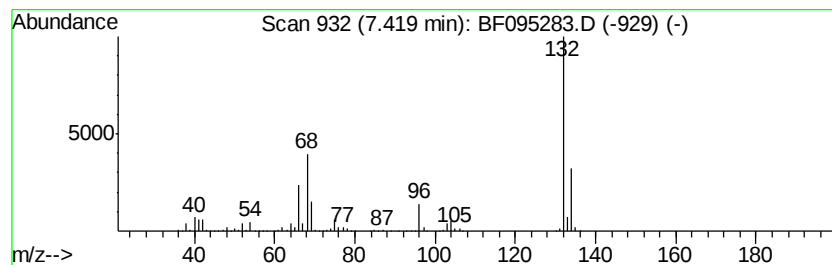
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Peak Number 2 unknown7.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	85.61 ng	2325870	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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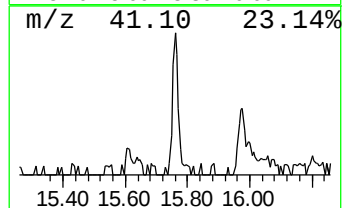
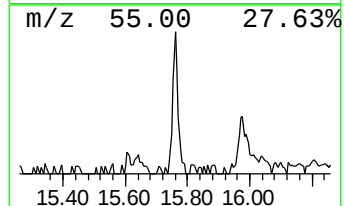
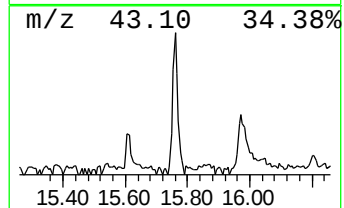
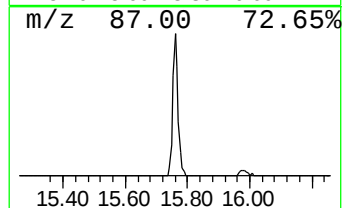
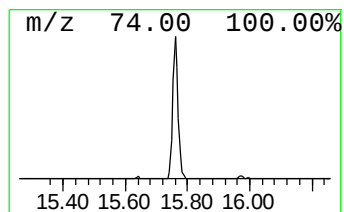
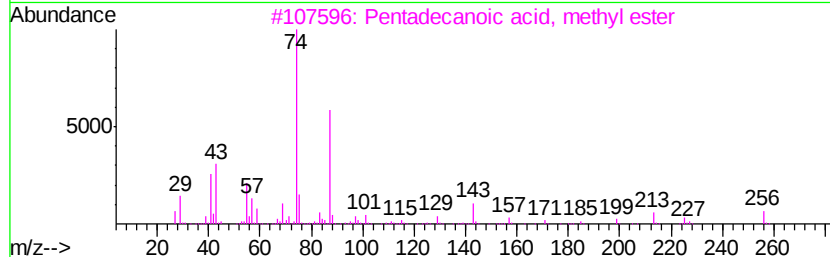
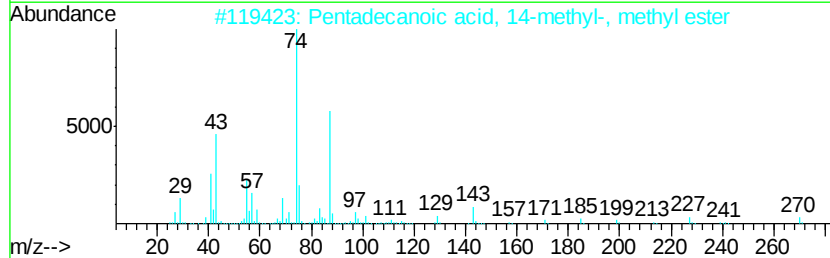
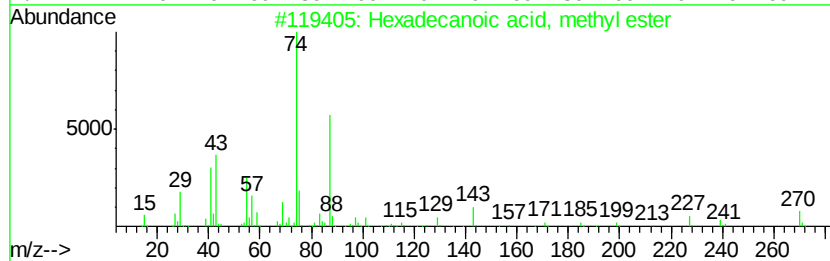
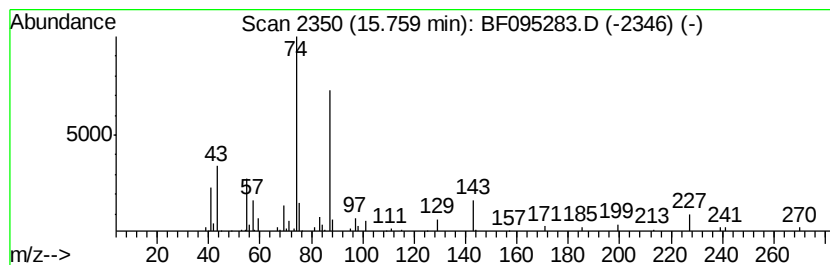
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Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.76	4.18 ng	128876	Phenanthrene-d10	15.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4		Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	83
5		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	80



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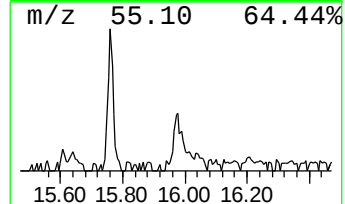
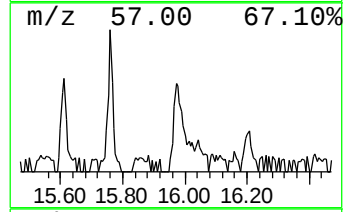
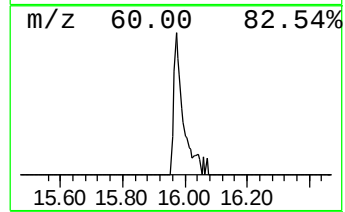
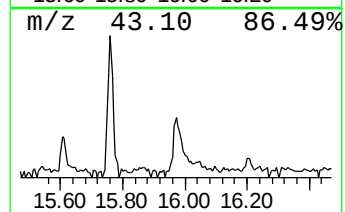
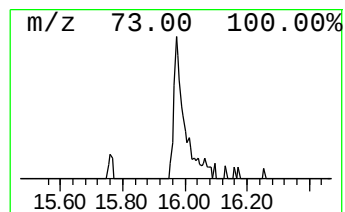
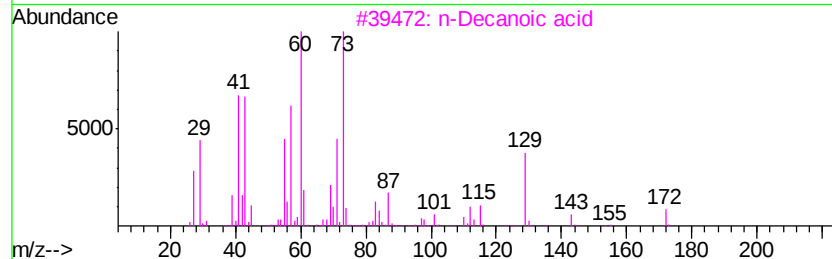
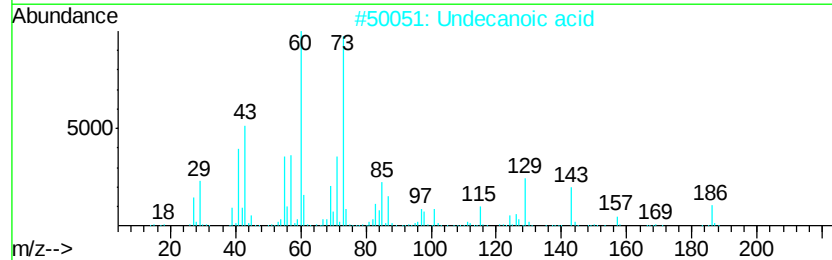
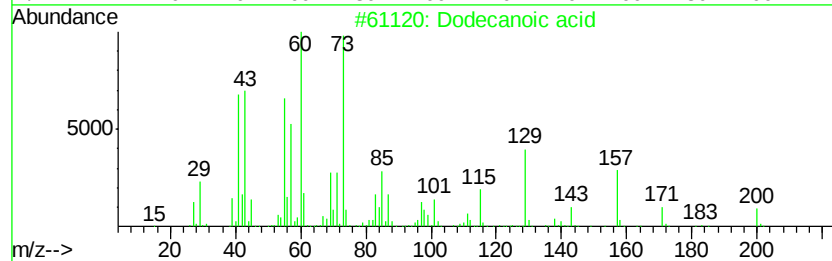
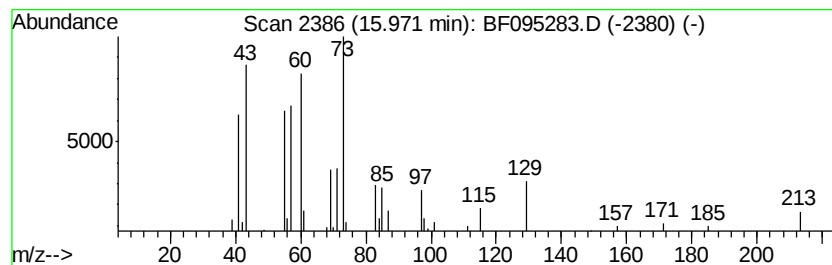
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Peak Number 5 Dodecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	2.50 ng	77178	Phenanthrene-d10	15.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	64	
2	Undecanoic acid	186	C11H22O2	000112-37-8	53	
3	n-Decanoic acid	172	C10H20O2	000334-48-5	47	
4	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	47	
5	.alpha.-d-Riboside, 1-O-dodecyl-	318	C17H34O5	1000154-76-8	43	



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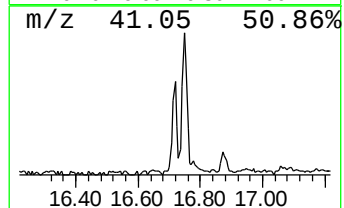
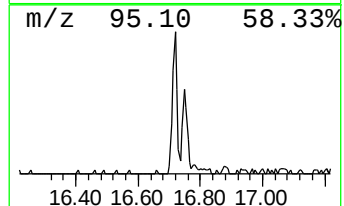
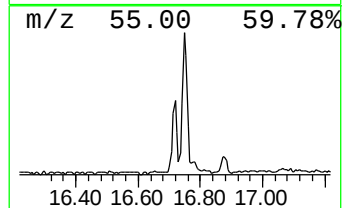
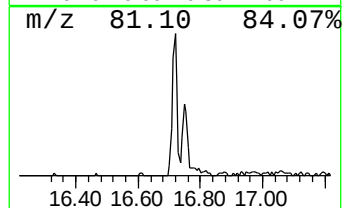
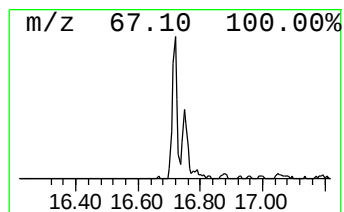
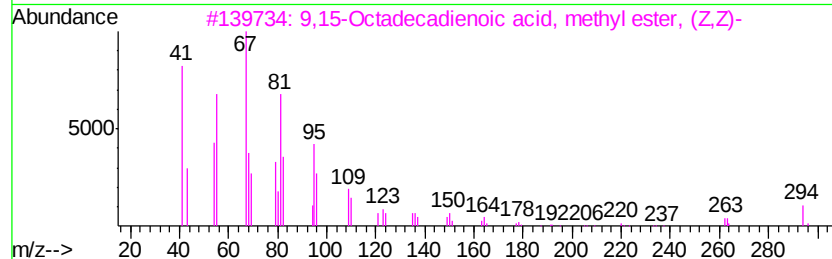
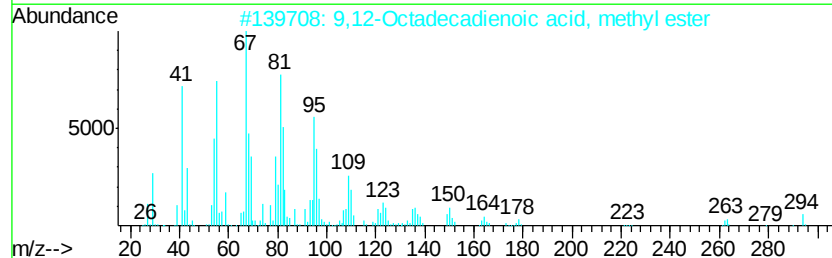
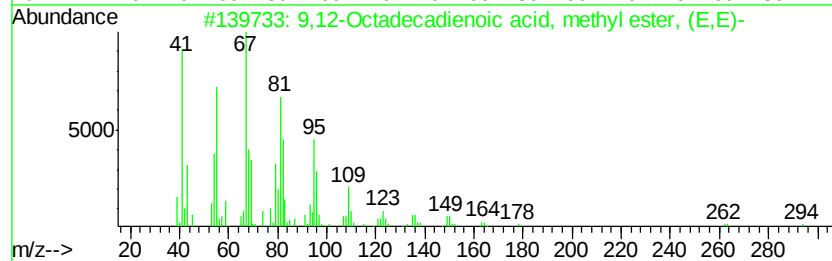
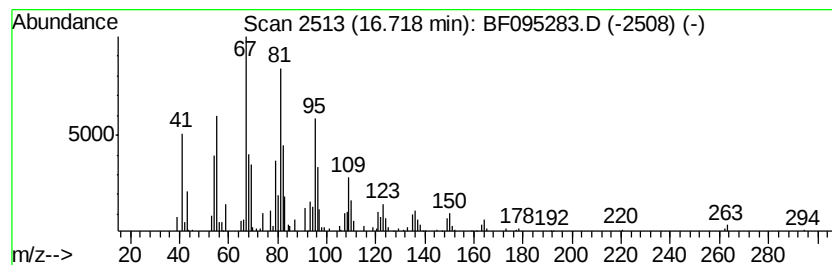
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Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	7.08 ng	218294	Phenanthrene-d10	15.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99		
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99		
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99		
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99		
5	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	95		



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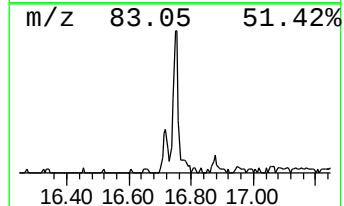
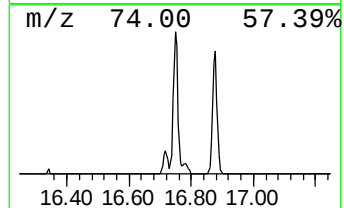
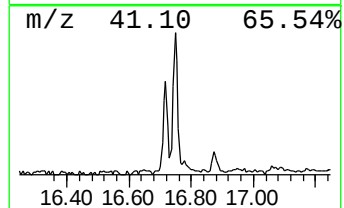
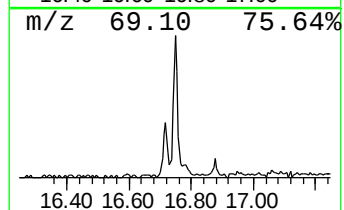
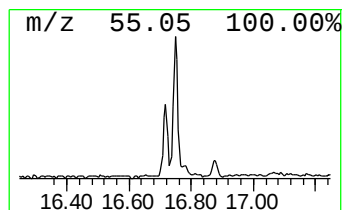
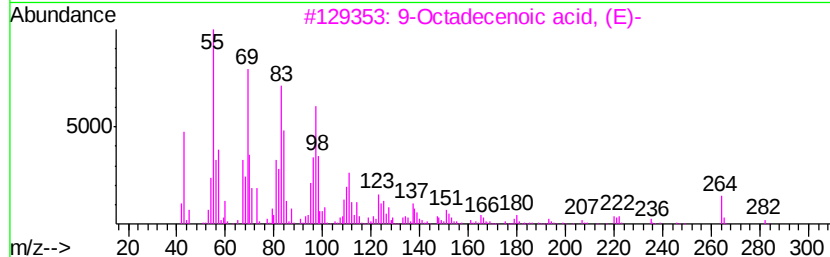
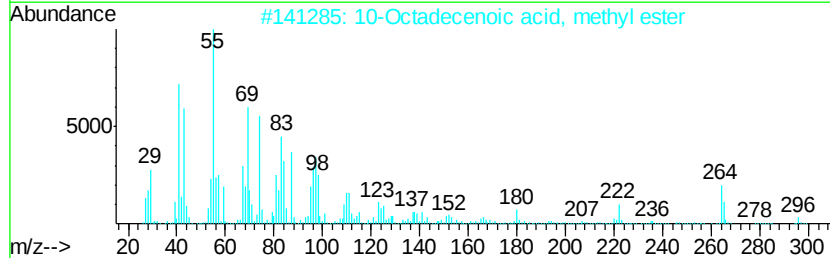
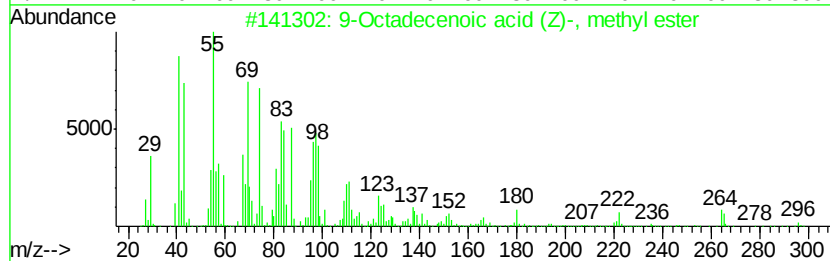
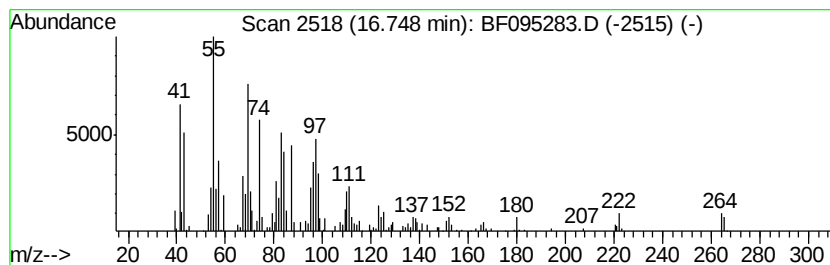
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BNA_F
ClientSampleId :
SB-3COMP

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 9-Octadecenoic acid (Z)-, m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.75	10.88 ng	335429	Phenanthrene-d10	15.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	83
3	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	81
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	70
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	70



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095283.D
Acq On : 20 May 2017 1:55
Operator : SJ/MA
Sample : I3202-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3COMP

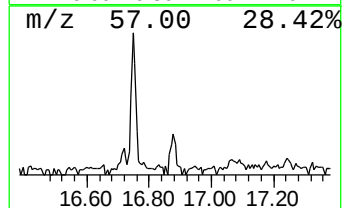
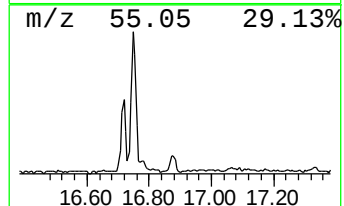
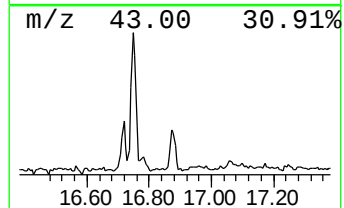
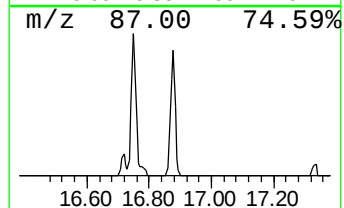
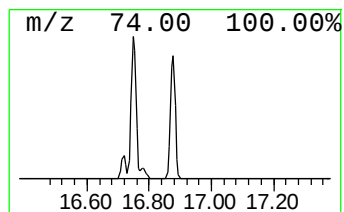
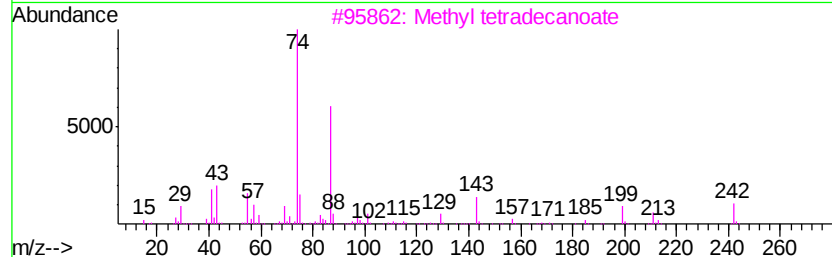
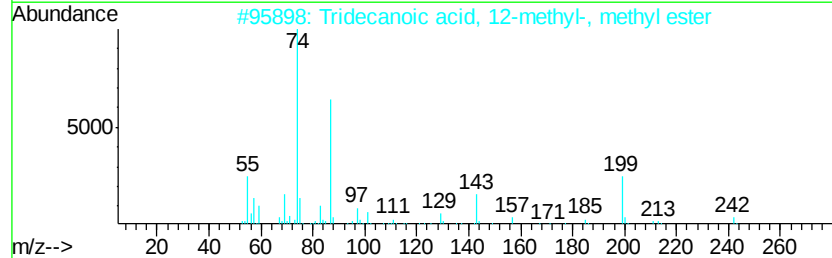
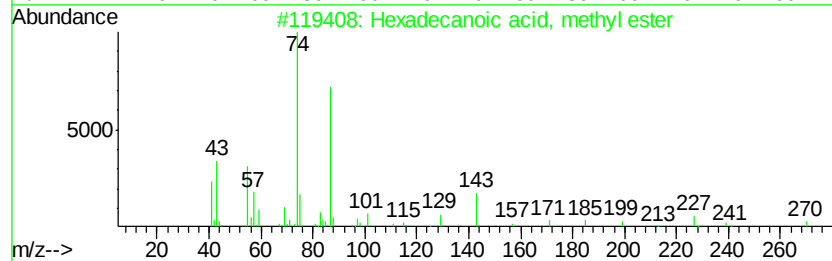
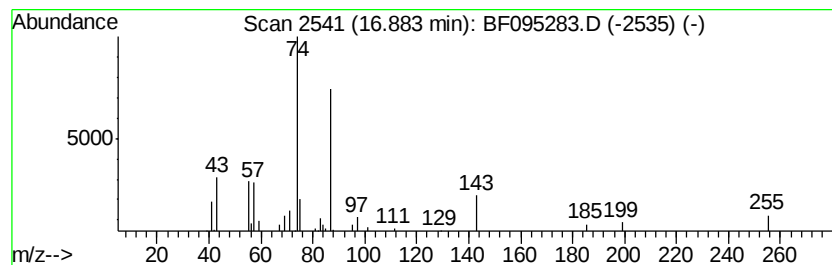
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecanoic acid, 12-methyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.88	2.48 ng	56928	Chrysene-d12	18.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	80
2		Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	78
3		Methyl tetradecanoate	242	C15H30O2	000124-10-7	78
4		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	72
5		Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
Data File : BF095283.D
Acq On : 20 May 2017 1:55
Operator : SJ/MA
Sample : I3202-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3COMP

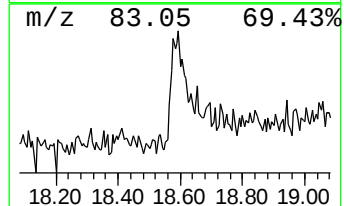
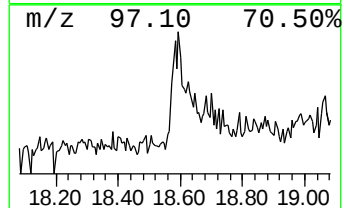
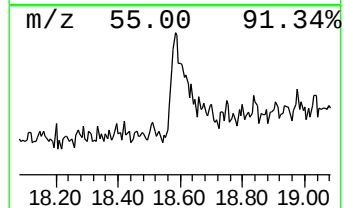
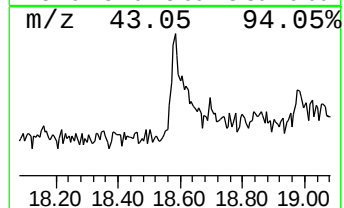
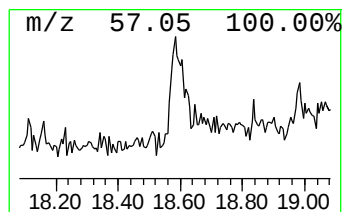
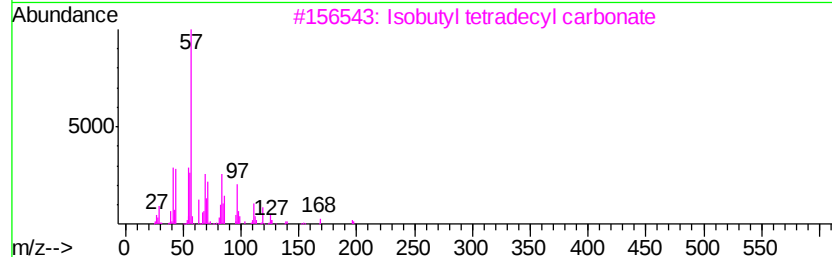
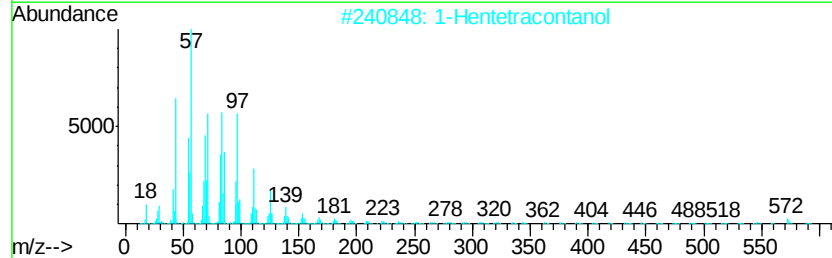
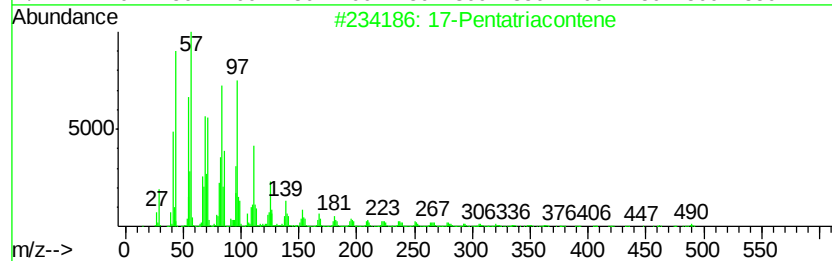
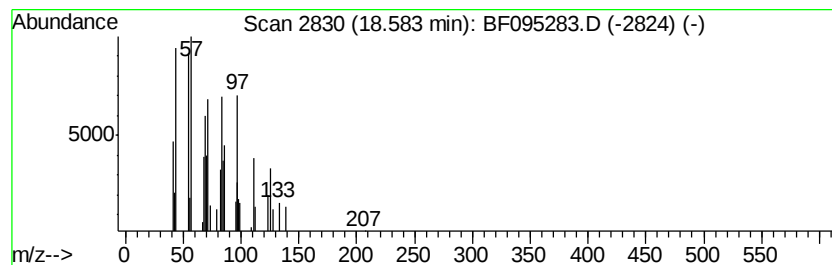
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	3.35 ng	76909	Chrysene-d12	18.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	87
2		1-Hentetracontanol	593	C41H84O	040710-42-7	86
3		Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	80
4		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	72
5		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051917\
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Acq On : 20 May 2017 1:55
Operator : SJ/MA
Sample : I3202-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3COMP

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.11	19.0	ng	516092	1	7.76	543345	20.0
unknown7.42	7.42	85.6	ng	2325870	1	7.76	543345	20.0
Hexadecanoic acid...	15.76	4.2	ng	128876	4	15.02	616409	20.0
Dodecanoic acid	15.97	2.5	ng	77178	4	15.02	616409	20.0
9,12-Octadecadien...	16.72	7.1	ng	218294	4	15.02	616409	20.0
9-Octadecenoic ac...	16.75	10.9	ng	335429	4	15.02	616409	20.0
Tridecanoic acid,...	16.88	2.5	ng	56928	5	18.69	458982	20.0
17-Pentatriacontene	18.58	3.4	ng	76909	5	18.69	458982	20.0