

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
 Data File : BF099557.D
 Acq On : 16 Oct 2017 21:22
 Operator : SJ/JU
 Sample : I5782-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S3(1-3)

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-BF092317.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	5.075	504	508	527	rBV	467802	662172	22.13%	2.578%
2	5.475	571	576	579	rBV	2523247	2528819	84.51%	9.846%
3	6.487	742	748	762	rBV	2327429	2741024	91.60%	10.673%
4	6.616	766	770	774	rBV	2665231	2691399	89.94%	10.479%
5	6.845	805	809	815	rBV	672652	588315	19.66%	2.291%
6	6.998	831	835	839	rBV	2255806	2094859	70.01%	8.157%
7	7.410	900	905	908	rBV	1634320	1686117	56.35%	6.565%
8	8.122	1022	1026	1030	rBV	831229	806894	26.96%	3.142%
9	9.198	1204	1209	1213	rBV	2898504	2992405	100.00%	11.651%
10	9.592	1272	1276	1285	rBV	719671	570164	19.05%	2.220%
11	9.880	1321	1325	1329	rBV	1050695	885527	29.59%	3.448%
12	10.592	1442	1446	1452	rBB	100488	78594	2.63%	0.306%
13	10.675	1455	1460	1463	rBV	1618536	1509651	50.45%	5.878%
14	11.369	1574	1578	1582	rBV	973923	814895	27.23%	3.173%
15	12.951	1843	1847	1851	rBV	2218298	2250687	75.21%	8.763%
16	13.833	1993	1997	2005	rBV	65738	91651	3.06%	0.357%
17	14.015	2024	2028	2035	rBV	597812	577226	19.29%	2.248%
18	14.457	2098	2103	2110	rBV4	27073	48737	1.63%	0.190%
19	14.762	2152	2155	2158	rVB	34578	34513	1.15%	0.134%
20	14.833	2163	2167	2173	rVB	345234	348326	11.64%	1.356%
21	14.910	2176	2180	2186	rBV	69786	79309	2.65%	0.309%
22	15.092	2208	2211	2214	rBV	80825	81800	2.73%	0.318%
23	15.486	2271	2278	2286	rBV2	467833	678923	22.69%	2.643%
24	15.668	2306	2309	2316	rVB4	22302	31526	1.05%	0.123%
25	15.898	2343	2348	2354	rVB	134294	187389	6.26%	0.730%
26	16.398	2427	2433	2441	rVB2	100671	175464	5.86%	0.683%
27	16.692	2479	2483	2488	rVB7	19938	36083	1.21%	0.140%
28	16.980	2526	2532	2540	rVB	76641	151694	5.07%	0.591%
29	17.245	2573	2577	2583	rBV7	21308	39158	1.31%	0.152%
30	17.674	2643	2650	2662	rVB2	50084	126731	4.24%	0.493%
31	18.492	2783	2789	2800	rVB5	29911	92864	3.10%	0.362%

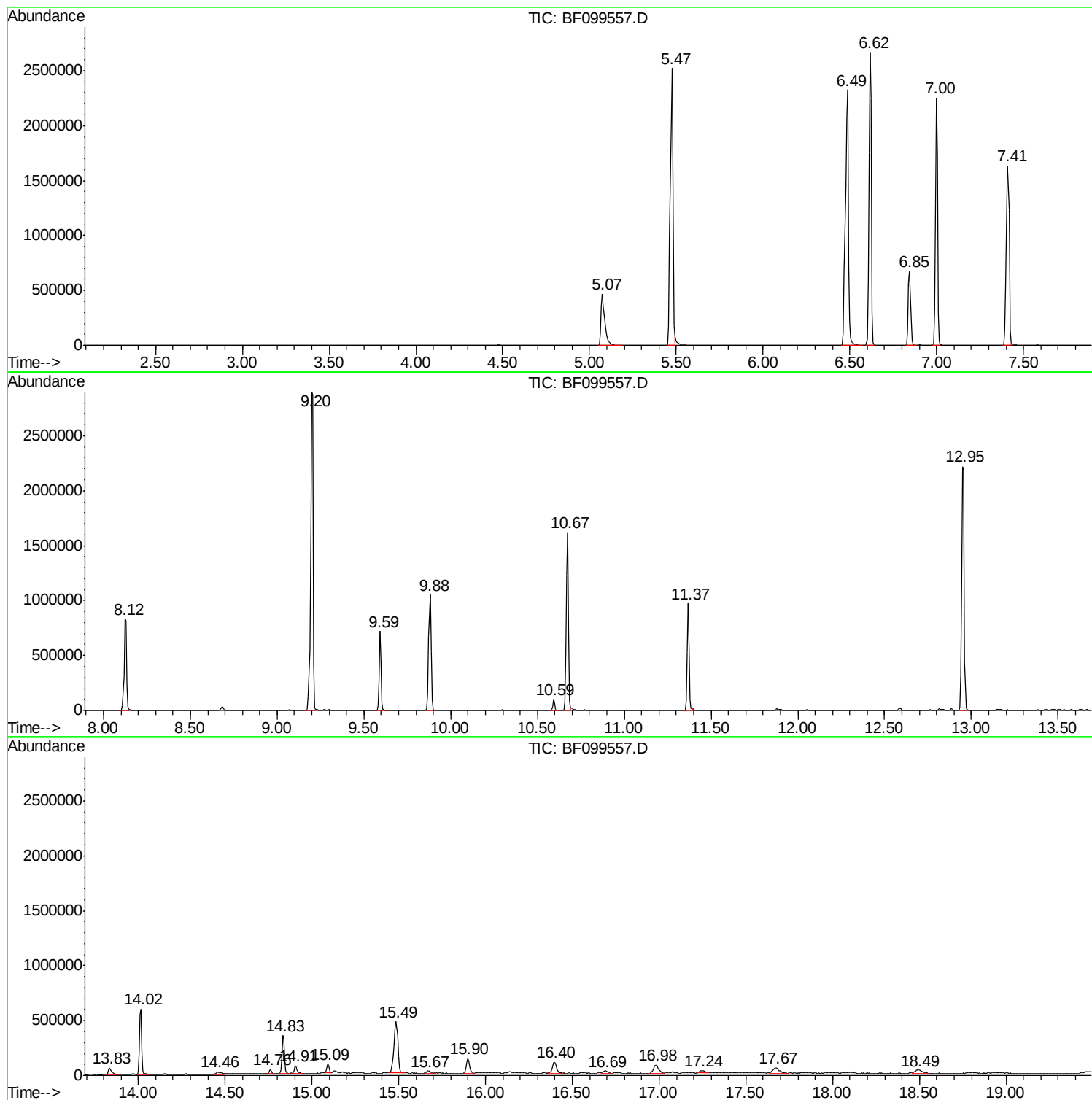
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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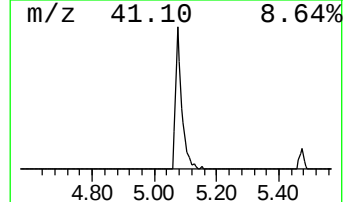
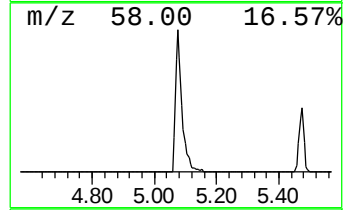
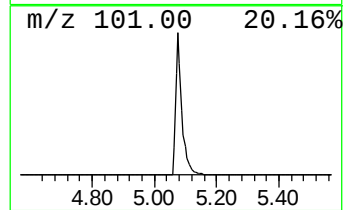
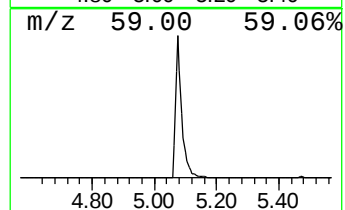
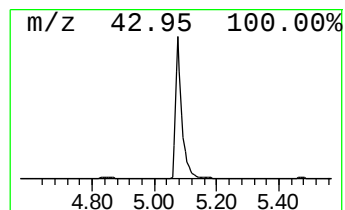
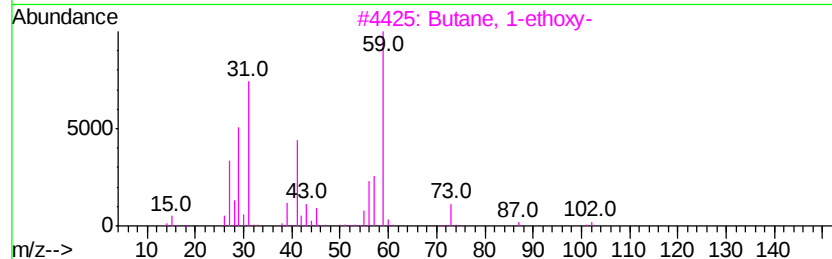
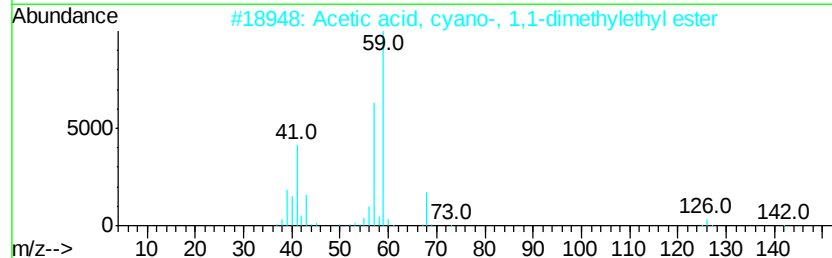
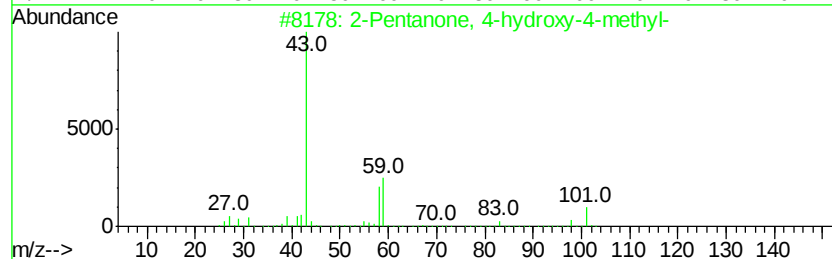
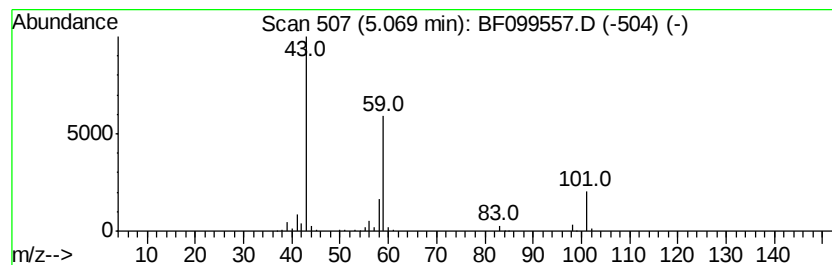
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	22.51 ng	662172	1,4-Dichlorobenzene-d4	6.85

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	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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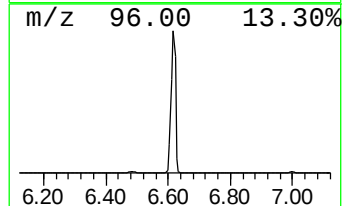
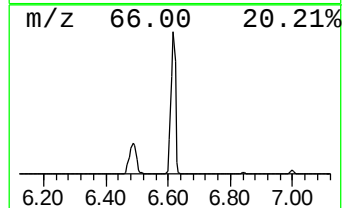
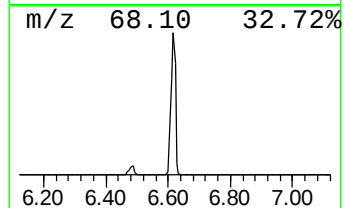
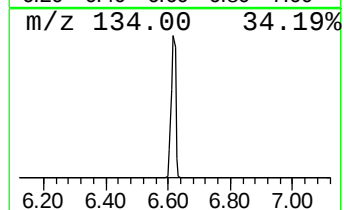
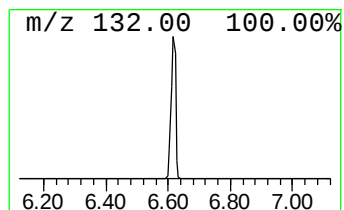
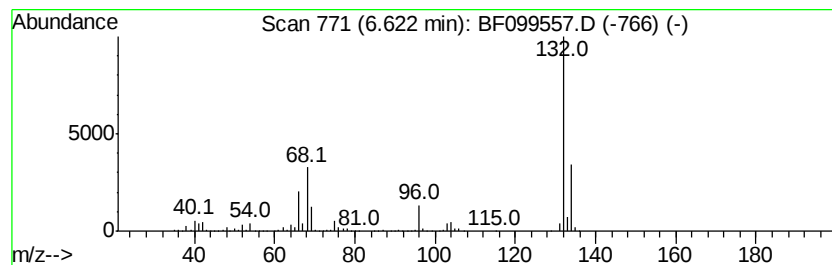
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	91.50 ng	2691400	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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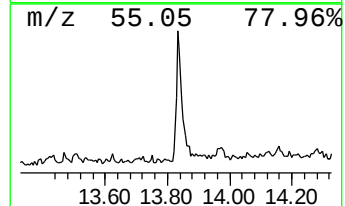
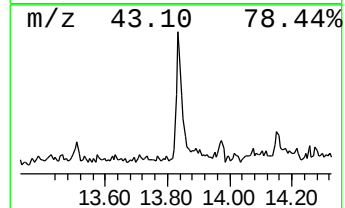
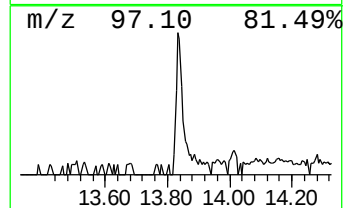
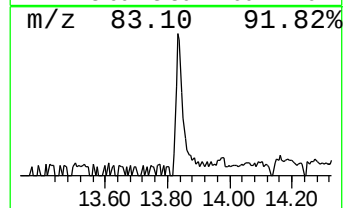
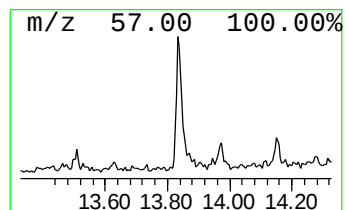
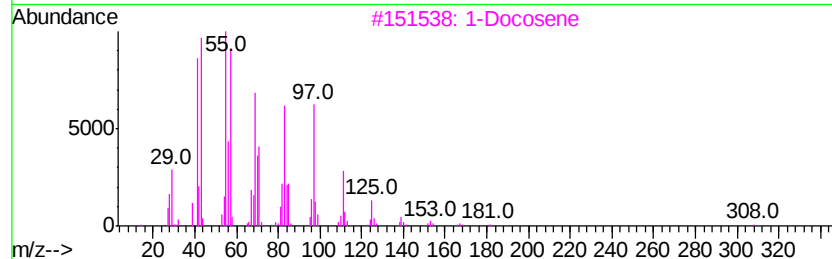
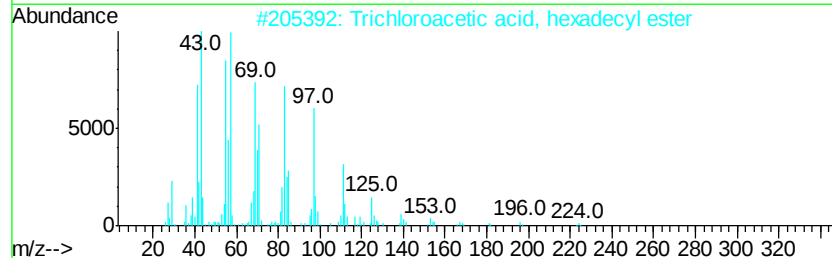
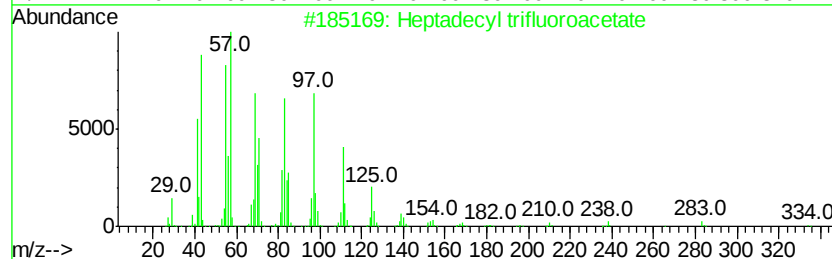
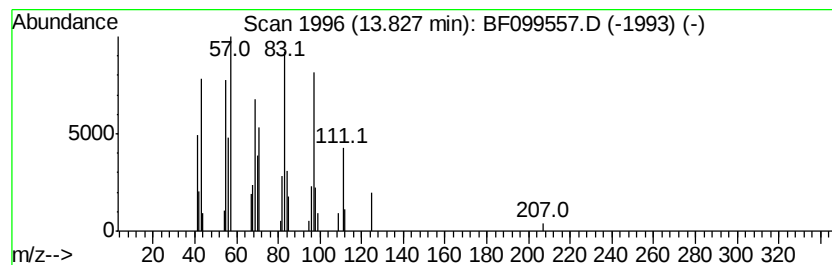
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Peak Number 4 Heptadecyl trifluoroacetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.18 ng	91651	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		1-Docosene	308	C22H44	001599-67-3	91
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



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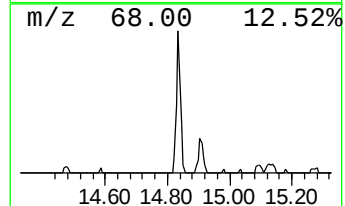
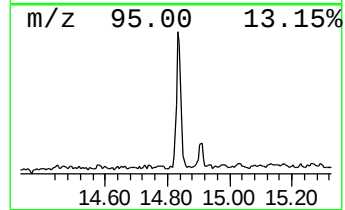
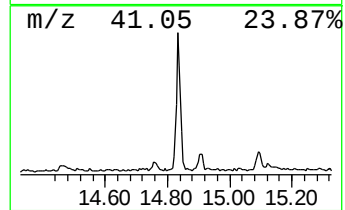
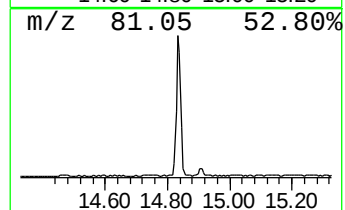
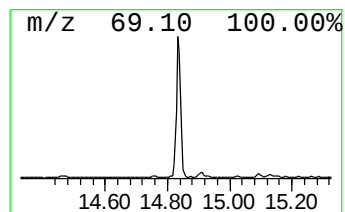
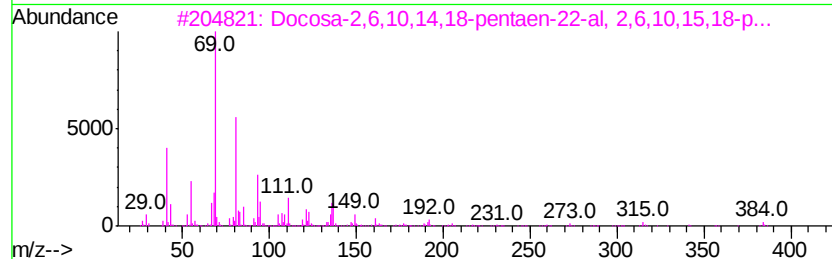
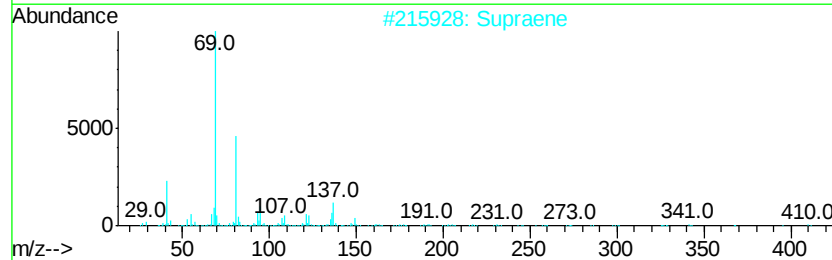
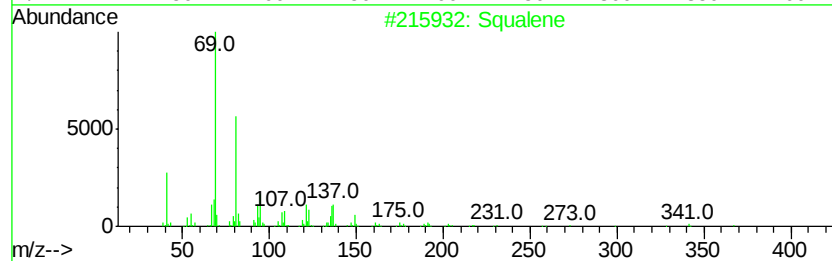
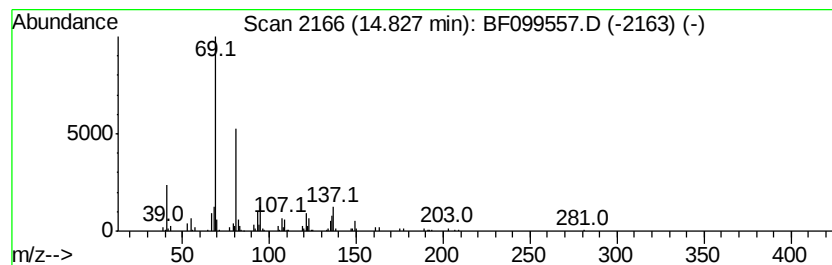
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Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	10.26 ng	348326	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4		2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	64
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64



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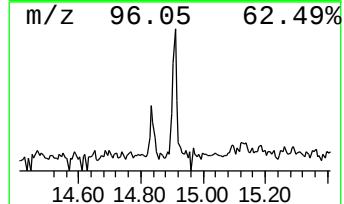
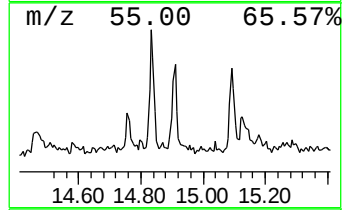
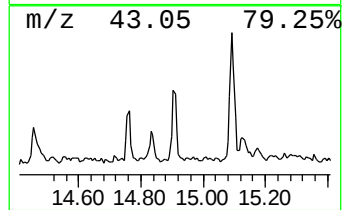
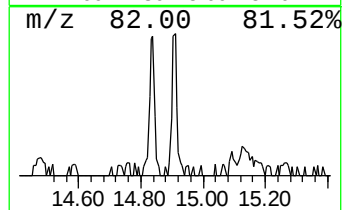
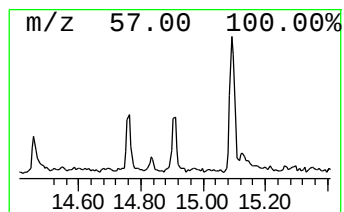
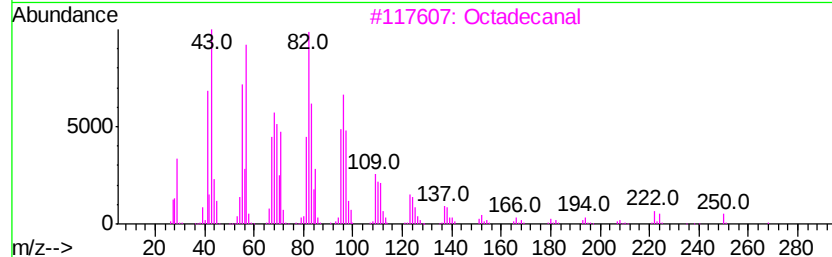
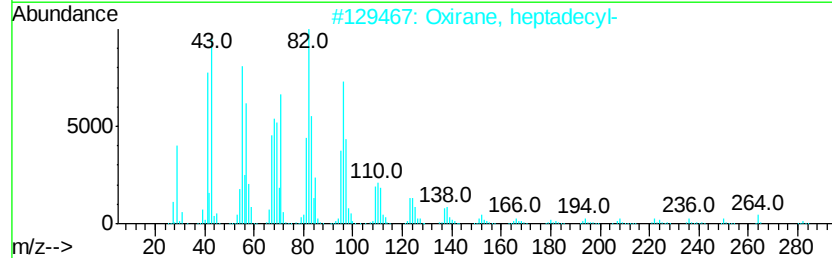
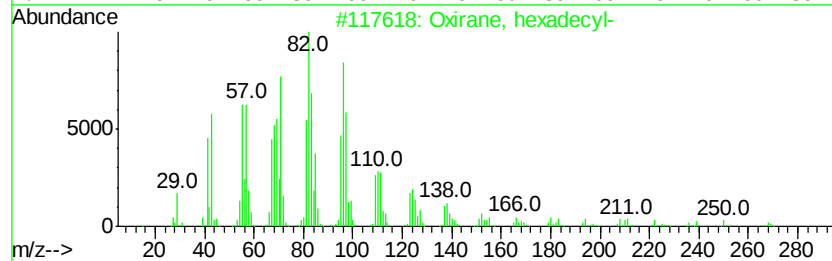
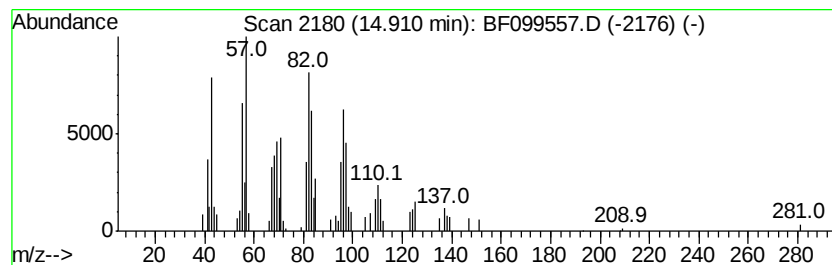
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Peak Number 6 Oxirane, hexadecyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.91	2.34 ng	79309	Perylene-d12		15.49
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
3	Octadecanal	268	C18H36O	000638-66-4	87
4	1,19-Eicosadiene	278	C20H38	014811-95-1	74
5	Hexadecanal	240	C16H32O	000629-80-1	64



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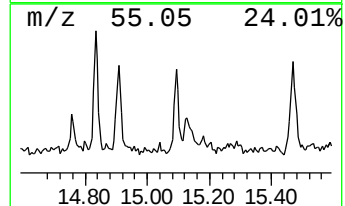
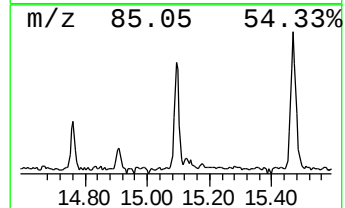
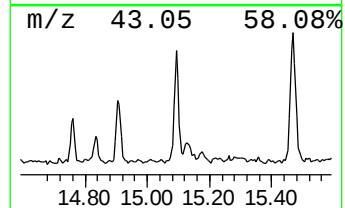
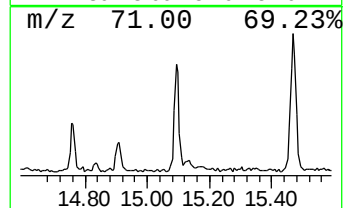
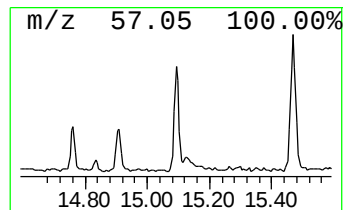
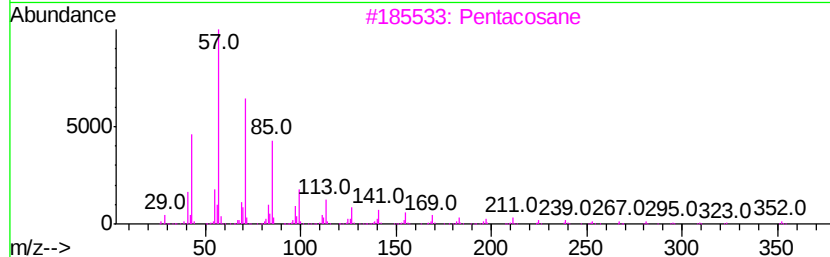
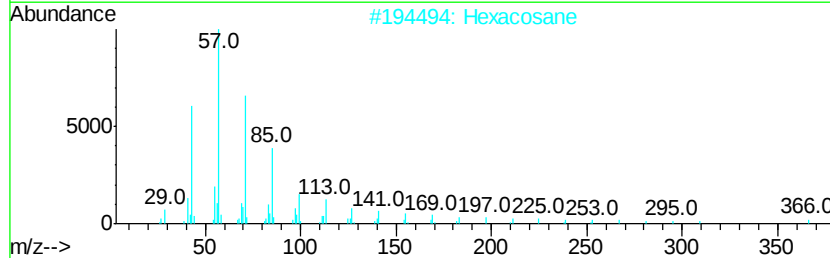
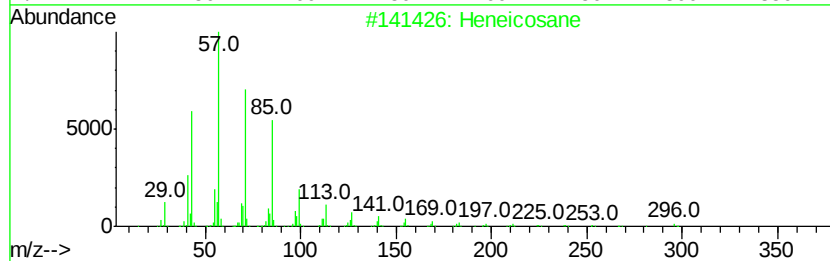
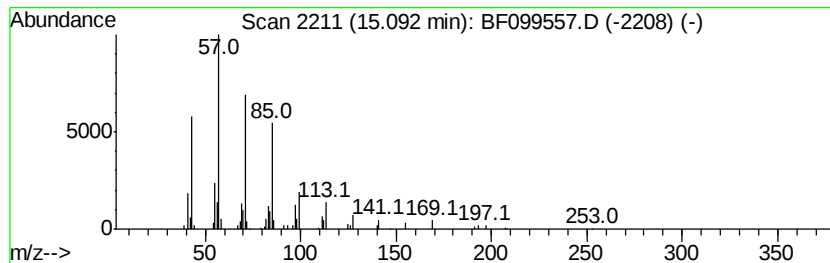
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	2.41 ng	81800	Perylene-d12	15.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Pentacosane		352	C25H52	000629-99-2	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	91
5	Octacosane		394	C28H58	000630-02-4	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
Data File : BF099557.D
Acq On : 16 Oct 2017 21:22
Operator : SJ/JU
Sample : I5782-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S3(1-3)

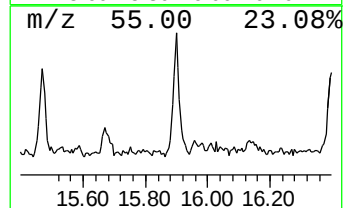
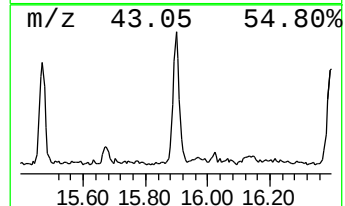
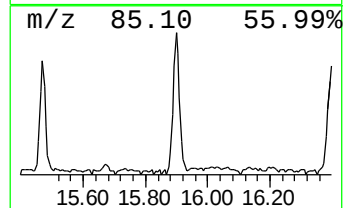
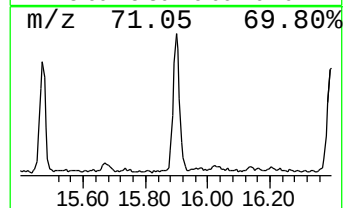
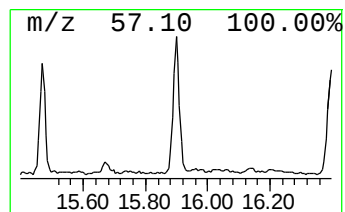
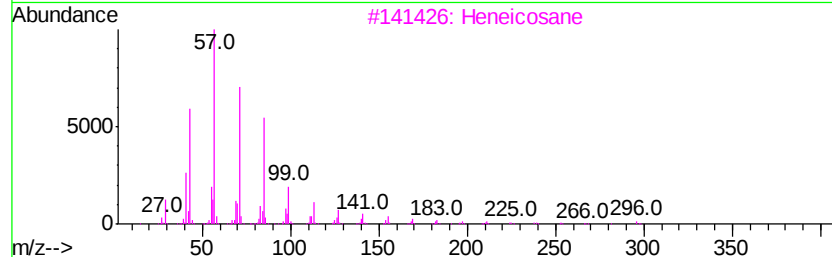
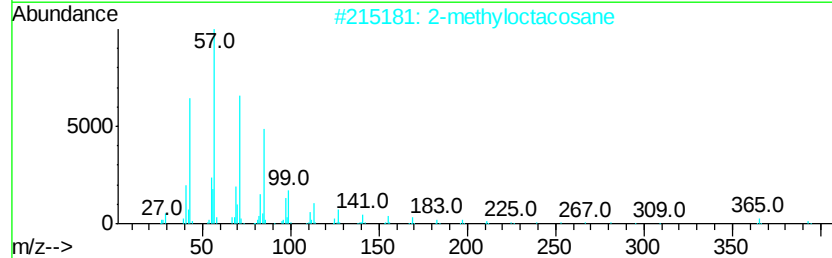
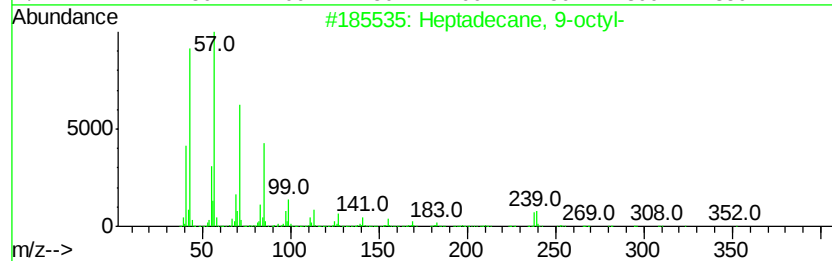
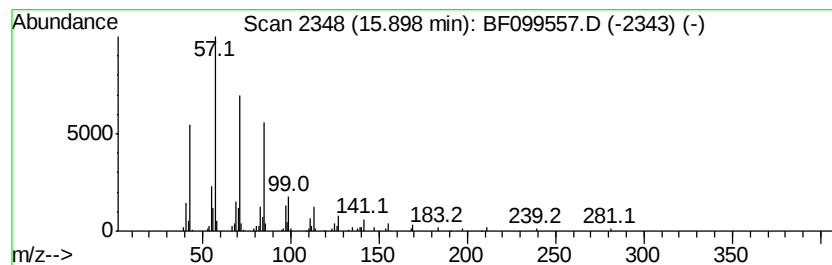
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	5.52 ng	187389	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Docosane	310	C22H46	000629-97-0	91
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
Data File : BF099557.D
Acq On : 16 Oct 2017 21:22
Operator : SJ/JU
Sample : I5782-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S3(1-3)

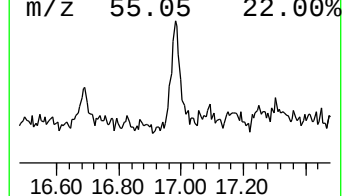
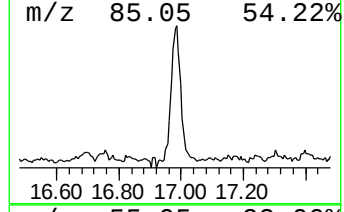
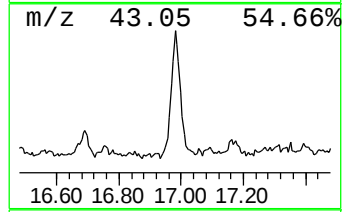
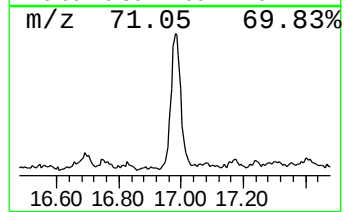
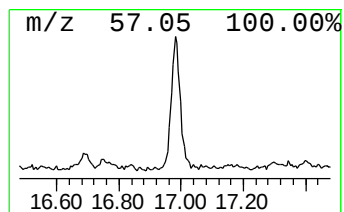
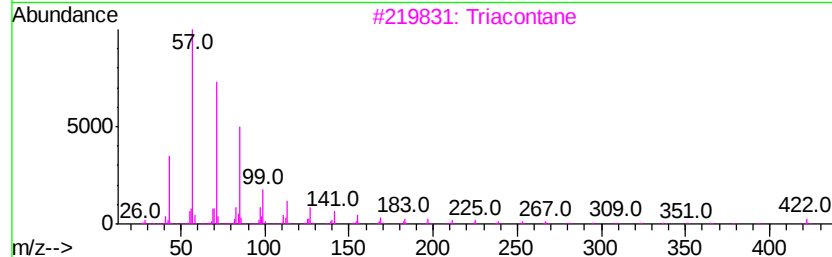
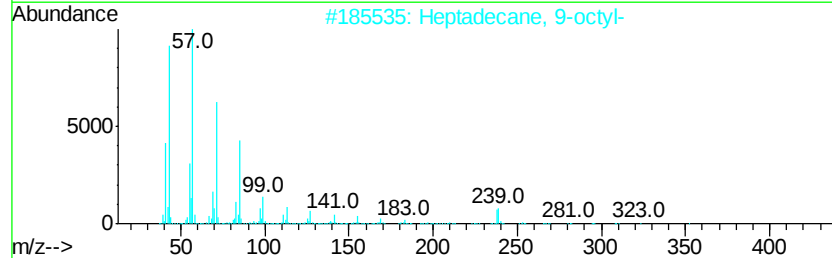
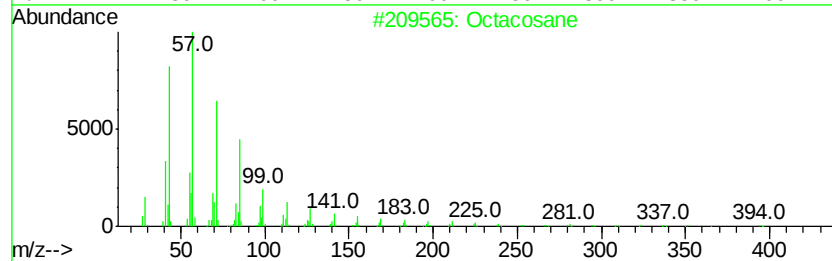
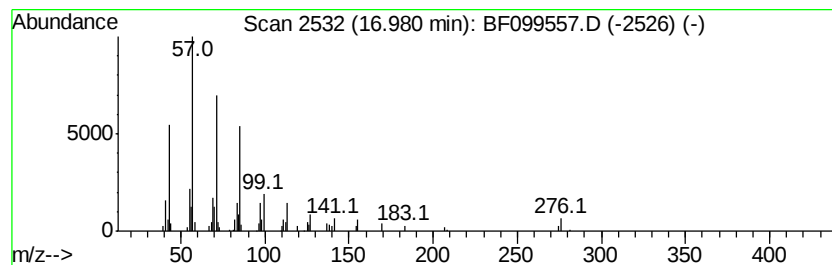
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.98	4.47 ng	151694	Perylene-d12	15.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Triacontane	422	C30H62	000638-68-6	91
4			2-methyloctacosane	408	C29H60	1000376-72-8	91
5			Pentacosane	352	C25H52	000629-99-2	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099557.D
Acq On : 16 Oct 2017 21:22
Operator : SJ/JU
Sample : I5782-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S3(1-3)

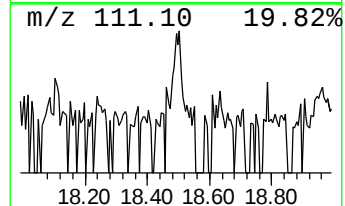
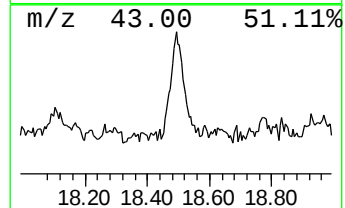
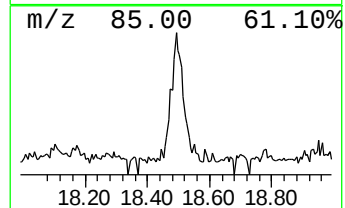
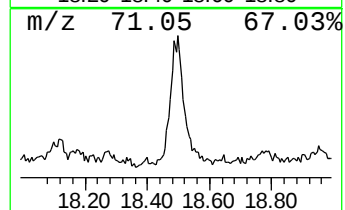
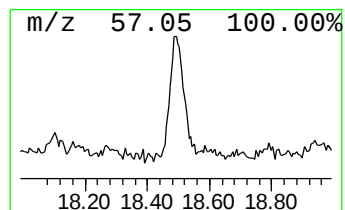
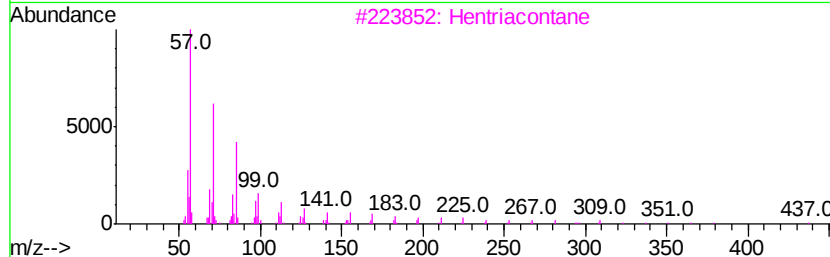
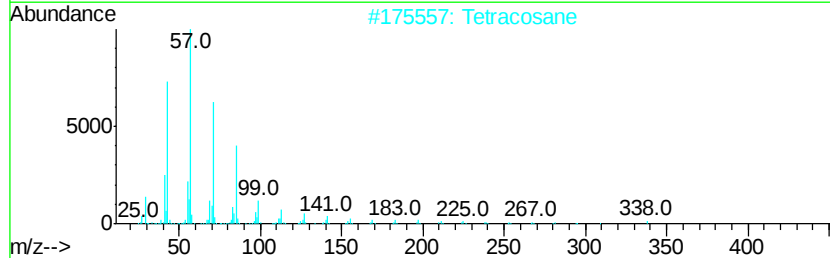
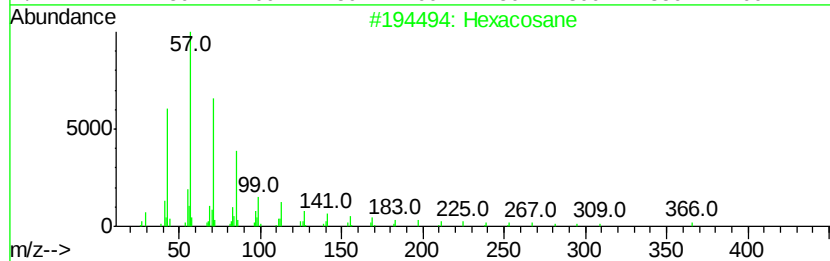
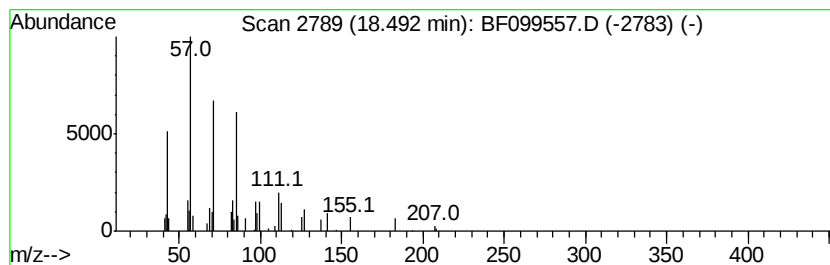
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.49	2.74 ng	92864	Perylene-d12	15.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	86
2			Tetracosane	338	C24H50	000646-31-1	80
3			Hentriacontane	437	C31H64	000630-04-6	80
4			Octacosane	394	C28H58	000630-02-4	80
5			Heptacosane	380	C27H56	000593-49-7	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
Data File : BF099557.D
Acq On : 16 Oct 2017 21:22
Operator : SJ/JU
Sample : I5782-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S3(1-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
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unknown6.62	6.62	91.5	ng	2691400	1	6.85	588315	20.0
Heptadecyl triflu...	13.83	3.2	ng	91651	5	14.02	577226	20.0
Squalene	14.83	10.3	ng	348326	6	15.49	678923	20.0
Oxirane, hexadecyl-	14.91	2.3	ng	79309	6	15.49	678923	20.0
Heneicosane	15.09	2.4	ng	81800	6	15.49	678923	20.0
Heptadecane, 9-oc...	15.90	5.5	ng	187389	6	15.49	678923	20.0
Octacosane	16.98	4.5	ng	151694	6	15.49	678923	20.0
Hexacosane	18.49	2.7	ng	92864	6	15.49	678923	20.0