

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082318\
 Data File : BF108446.D
 Acq On : 24 Aug 2018 3:43
 Operator : JU/SJ
 Sample : J4546-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BRICK-WALL-BPM

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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	2.384	3	8	15	rVB	323639	462435	13.55%	1.591%
2	5.254	491	496	511	rVB	96146	133794	3.92%	0.460%
3	5.631	555	560	563	rBV	3037134	3074548	90.08%	10.576%
4	6.625	723	729	732	rBV	3081059	3247678	95.15%	11.171%
5	6.772	749	754	757	rBV	3395611	3269288	95.78%	11.246%
6	7.001	789	793	796	rBV	1017258	853974	25.02%	2.937%
7	7.160	815	820	823	rBV	2518378	2492083	73.01%	8.572%
8	7.566	883	889	892	rBV	1989770	2096033	61.41%	7.210%
9	8.283	1006	1011	1030	rVB	1236434	1068151	31.29%	3.674%
10	9.360	1188	1194	1197	rBV	3669048	3413265	100.00%	11.741%
11	9.748	1256	1260	1265	rBV	190200	181290	5.31%	0.624%
12	10.042	1306	1310	1320	rVB	1218312	1156703	33.89%	3.979%
13	10.836	1441	1445	1458	rBV	1884607	1730395	50.70%	5.952%
14	11.542	1561	1565	1568	rBV	1079182	996436	29.19%	3.428%
15	12.924	1796	1800	1803	rBV	165686	139427	4.08%	0.480%
16	13.001	1810	1813	1816	rVB2	39568	35140	1.03%	0.121%
17	13.124	1830	1834	1837	rBV	2650633	2314578	67.81%	7.962%
18	13.630	1917	1920	1923	rVB	105303	82483	2.42%	0.284%
19	13.677	1923	1928	1930	rBV	57751	57152	1.67%	0.197%
20	14.001	1980	1983	1987	rBV	64562	59273	1.74%	0.204%
21	14.112	1994	2002	2012	rBV8	46654	201827	5.91%	0.694%
22	14.189	2012	2015	2022	rVB	814236	790305	23.15%	2.718%
23	14.318	2034	2037	2041	rBV	86664	76378	2.24%	0.263%
24	14.624	2086	2089	2093	rVB	79903	81360	2.38%	0.280%
25	14.954	2141	2145	2149	rBV	81883	86957	2.55%	0.299%
26	15.312	2203	2206	2211	rVB	63575	78541	2.30%	0.270%
27	15.748	2272	2280	2290	rBV	525272	759535	22.25%	2.613%
28	16.201	2352	2357	2362	rVB2	46983	71215	2.09%	0.245%
29	16.748	2446	2450	2462	rVB3	28597	61297	1.80%	0.211%

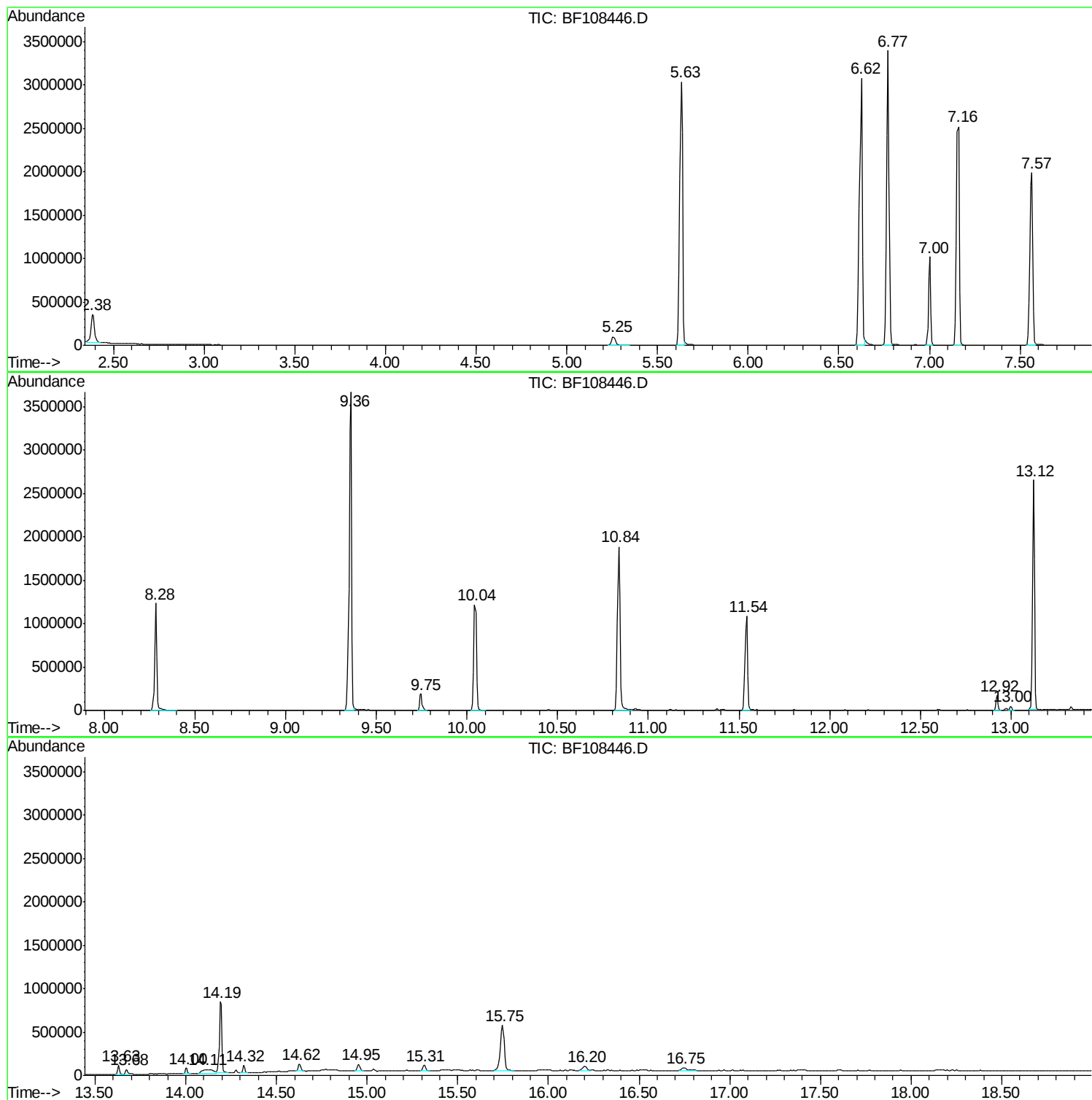
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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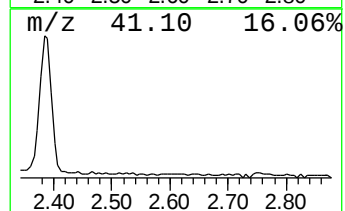
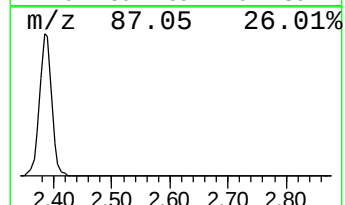
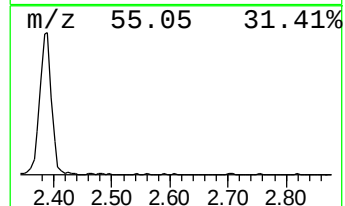
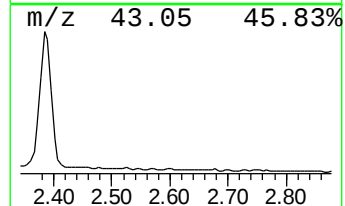
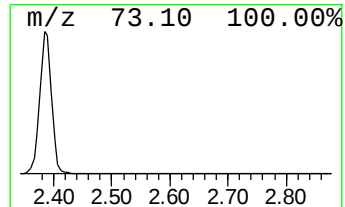
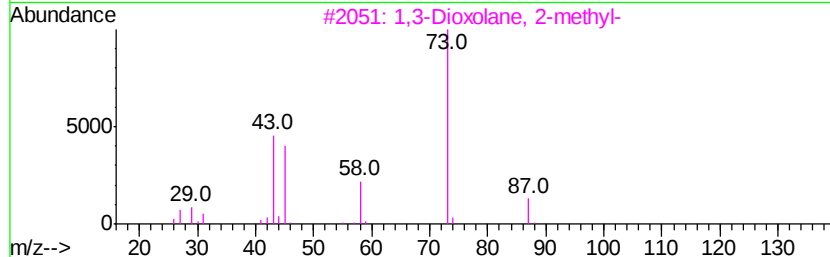
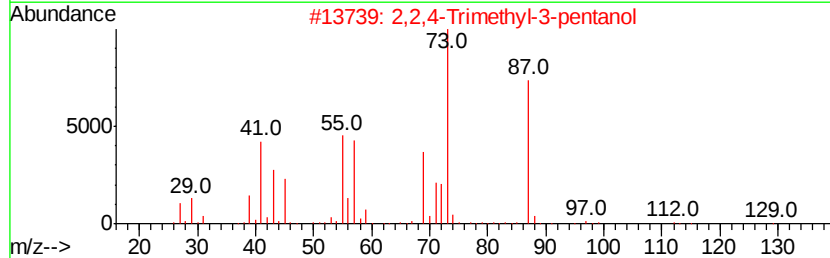
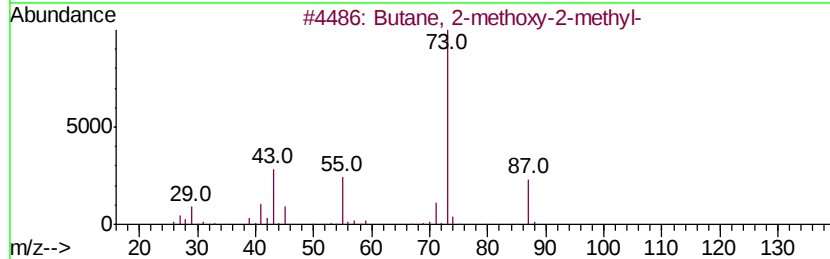
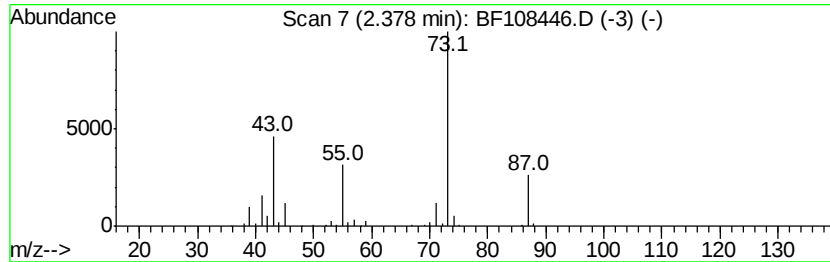
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.38	10.83 ng	462435	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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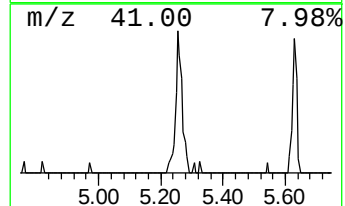
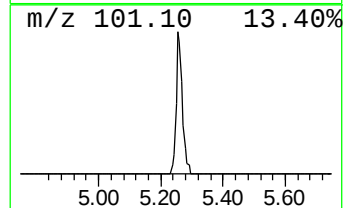
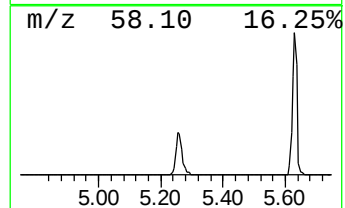
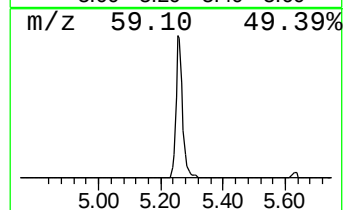
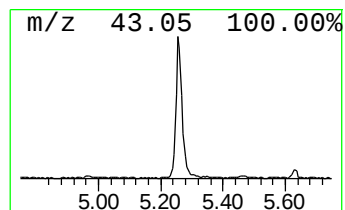
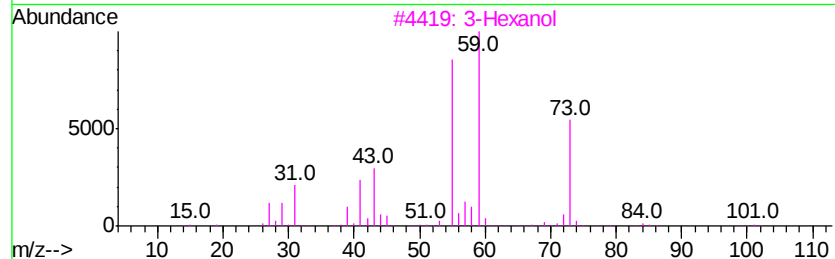
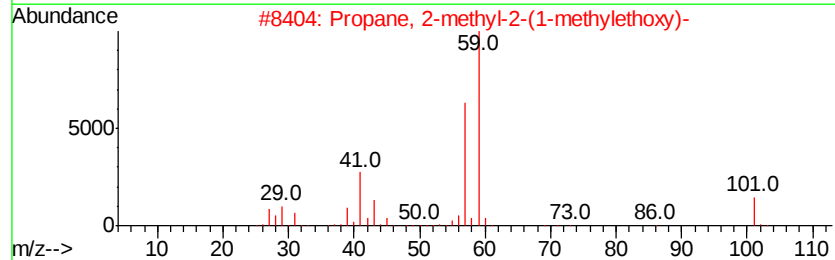
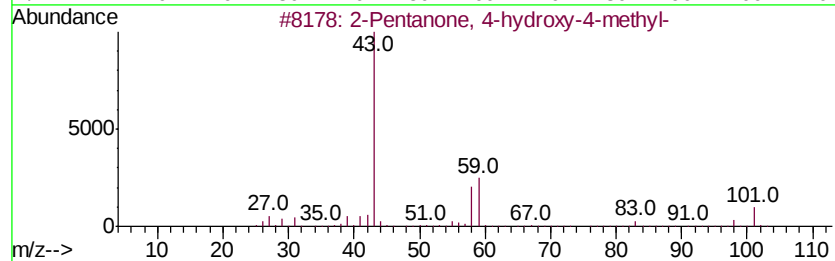
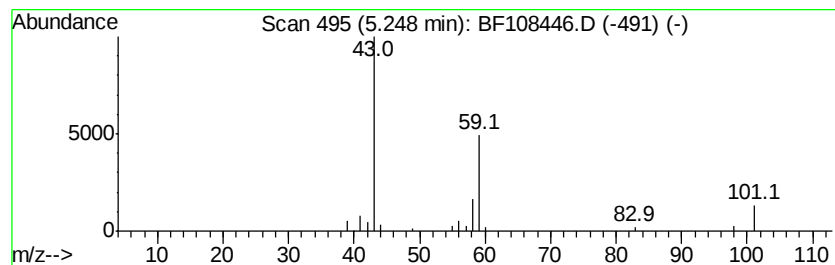
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	3.13 ng	133794	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol	102	C6H14O	000623-37-0	25
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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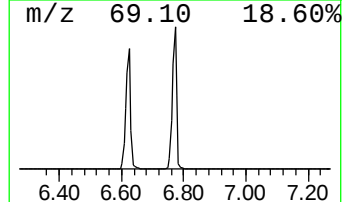
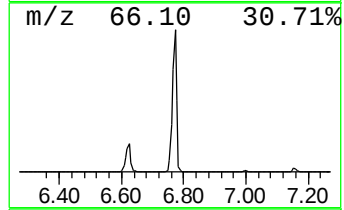
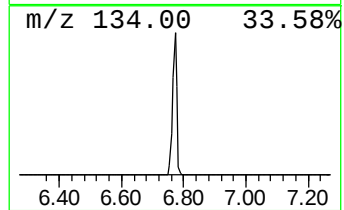
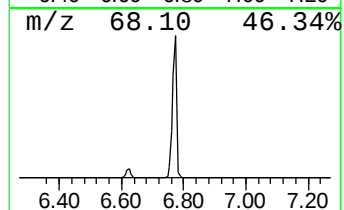
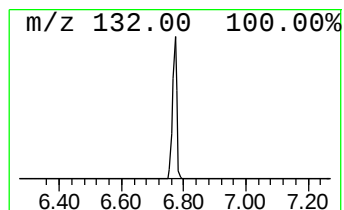
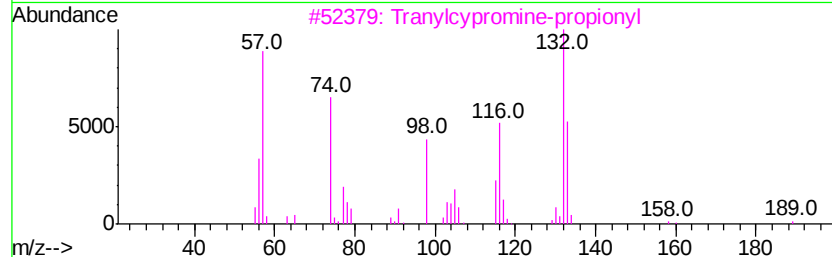
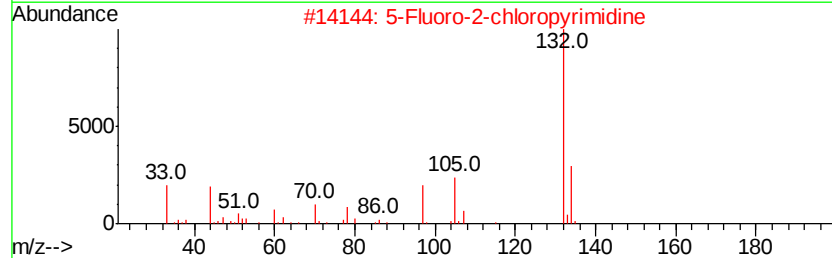
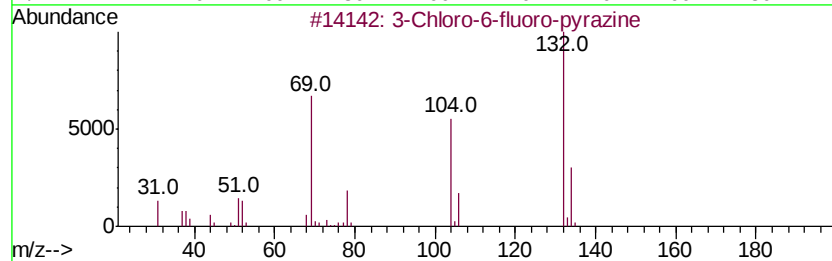
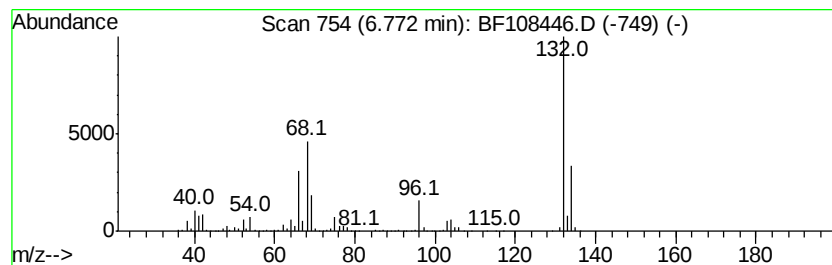
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Peak Number 3 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	76.57 ng	3269290	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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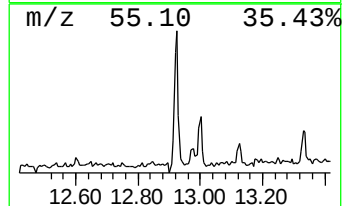
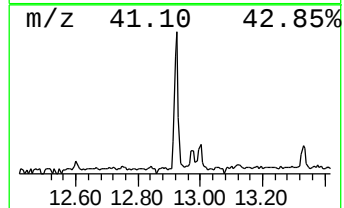
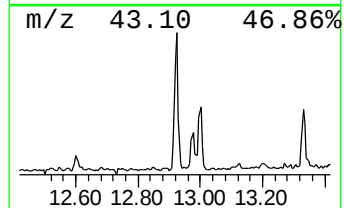
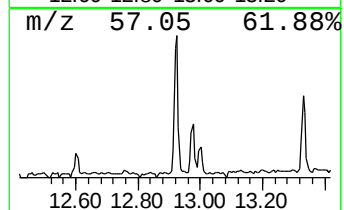
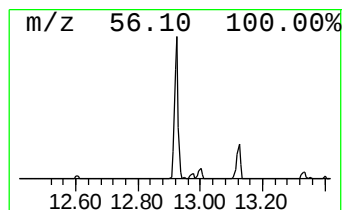
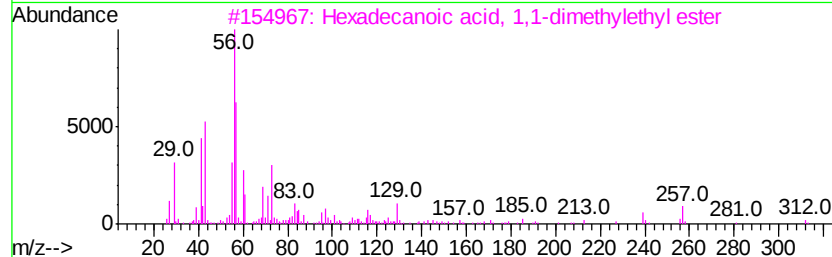
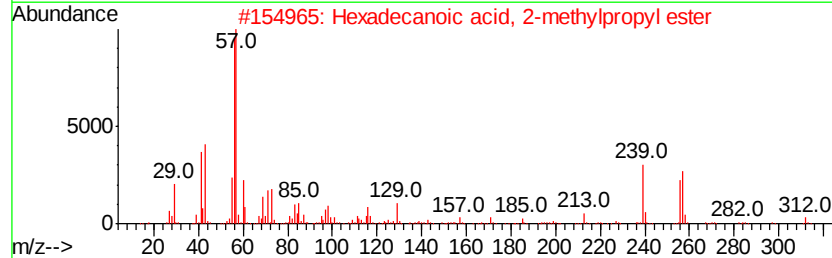
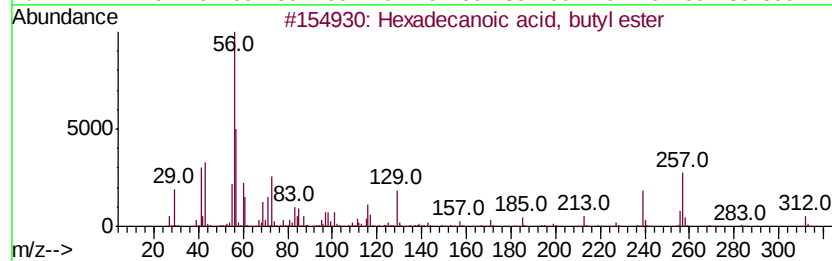
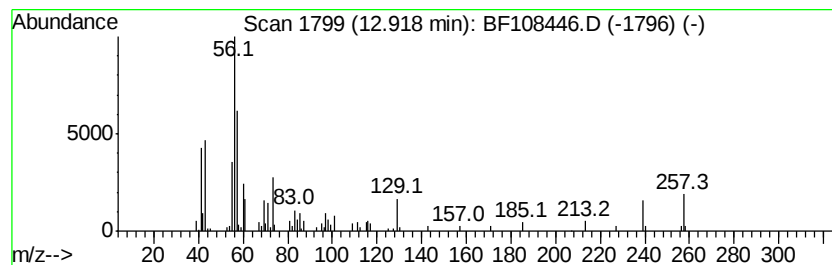
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.92	3.53 ng	139427	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 2-methylpropyl ester	312	C20H40O2	000110-34-9	64
3		Hexadecanoic acid, 1,1-dimethylethyl ester	312	C20H40O2	031158-91-5	55
4		Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	42
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35



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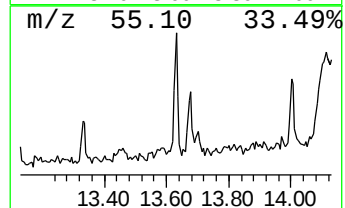
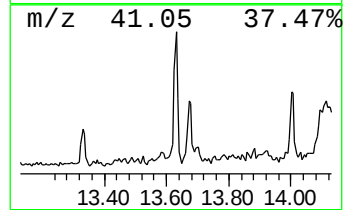
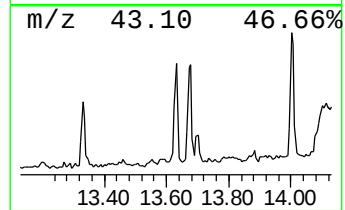
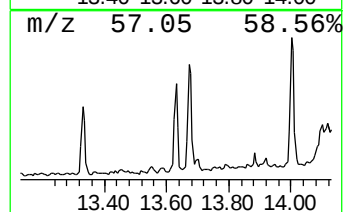
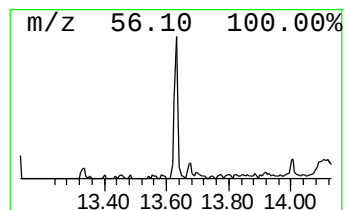
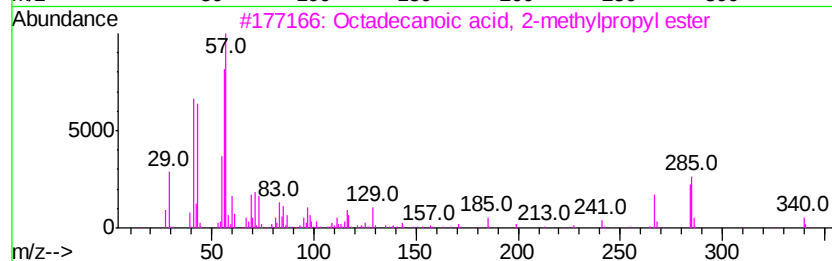
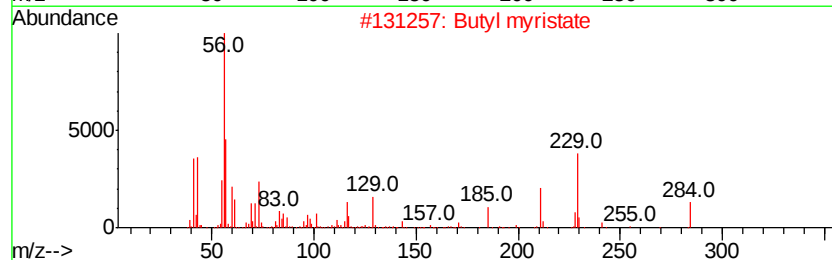
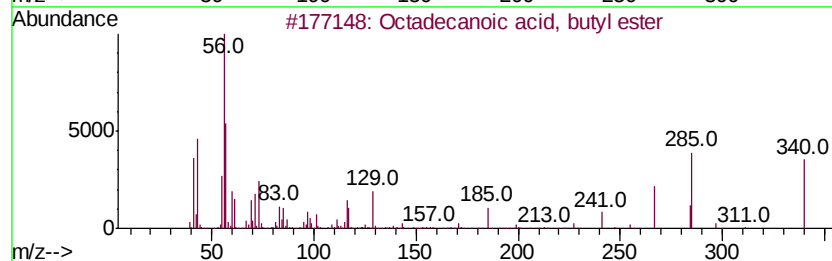
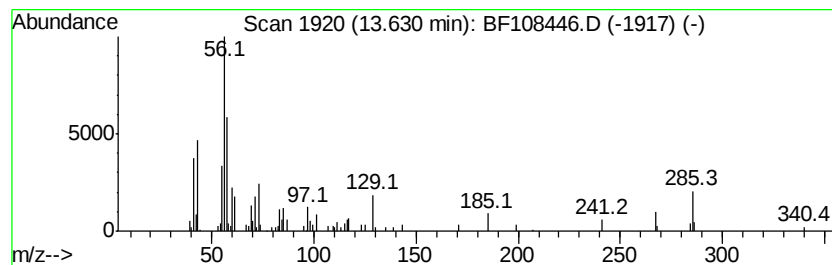
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Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	2.09 ng	82483	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2		Butyl myristate	284	C18H36O2	000110-36-1	59
3		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	47
4		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	37
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35



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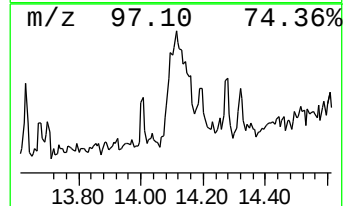
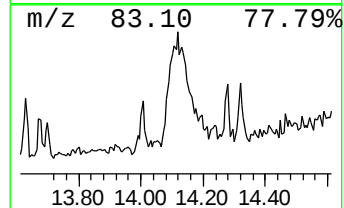
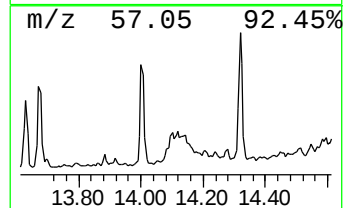
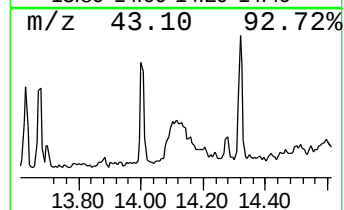
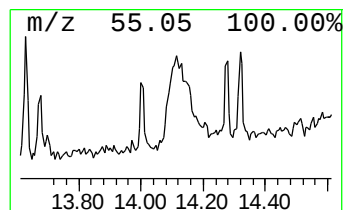
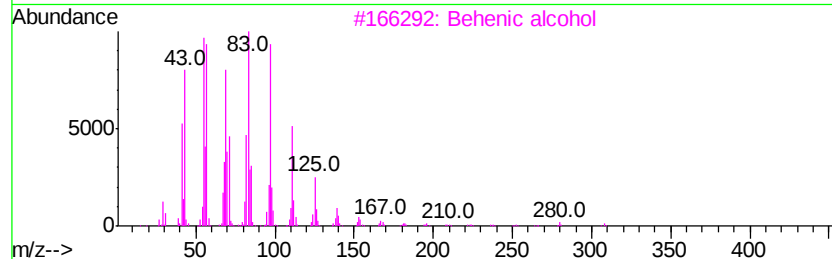
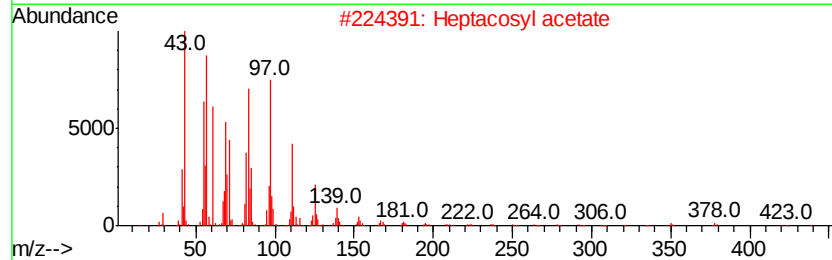
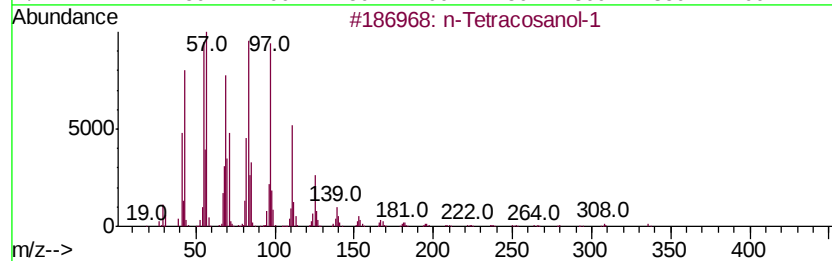
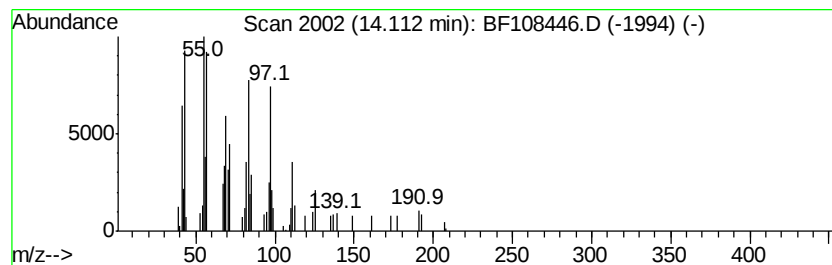
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BNA_F
ClientSampleId :
BRICK-WALL-BPM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.11	5.11 ng	201827	Chrysene-d12		14.19
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	Heptacosyl acetate	438	C29H58O2	1000351-78-2	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5	Octacosanol	410	C28H58O	000557-61-9	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082318\
Data File : BF108446.D
Acq On : 24 Aug 2018 3:43
Operator : JU/SJ
Sample : J4546-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BRICK-WALL-BPM

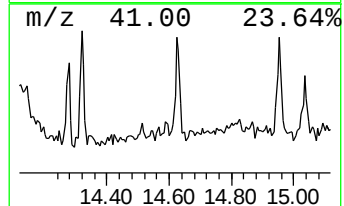
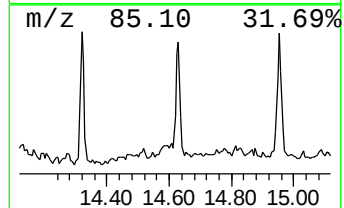
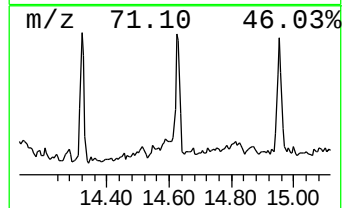
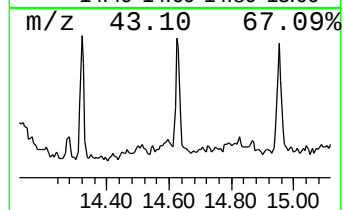
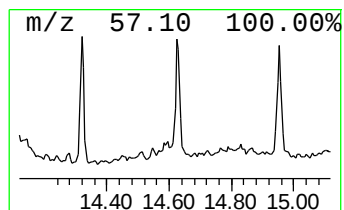
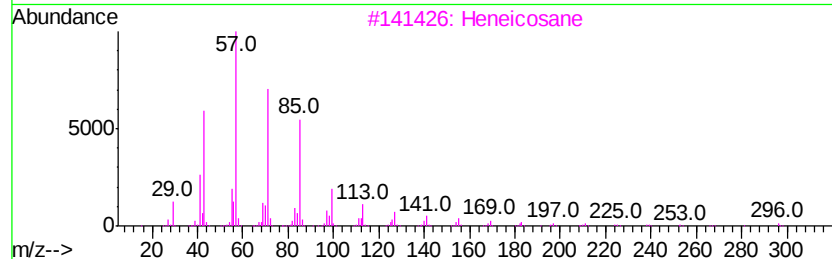
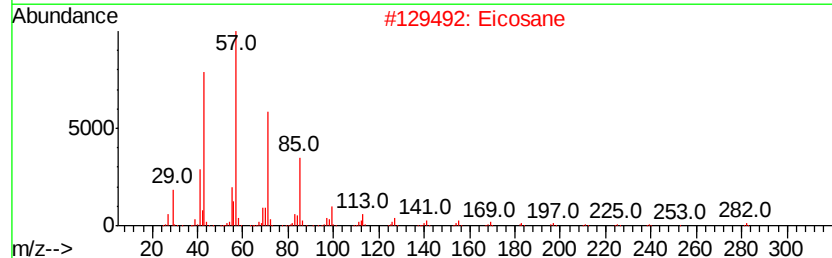
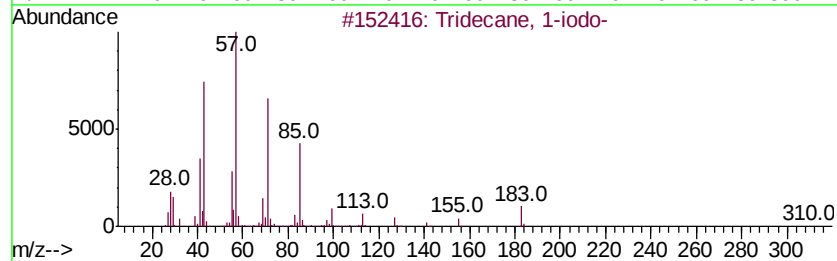
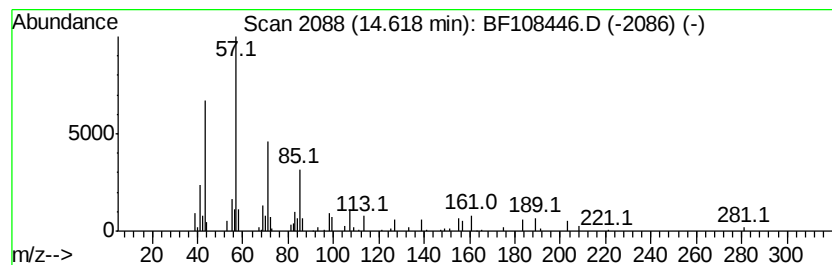
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecane, 1-iodo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.06 ng	81360	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
2		Eicosane	282	C20H42	000112-95-8	87
3		Heneicosane	296	C21H44	000629-94-7	87
4		Hexacosane	366	C26H54	000630-01-3	86
5		Octadecane	254	C18H38	000593-45-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082318\
Data File : BF108446.D
Acq On : 24 Aug 2018 3:43
Operator : JU/SJ
Sample : J4546-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BRICK-WALL-BPM

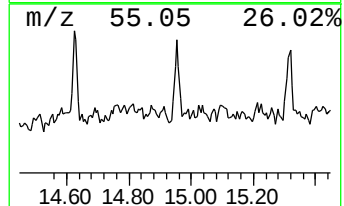
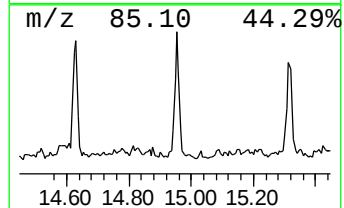
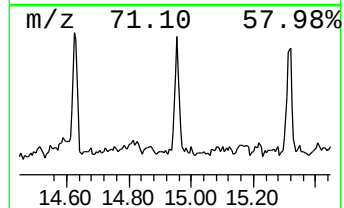
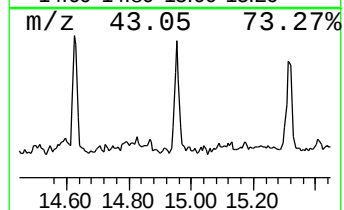
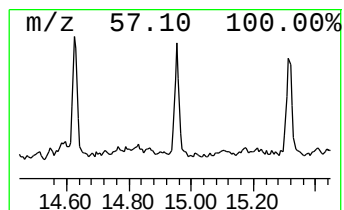
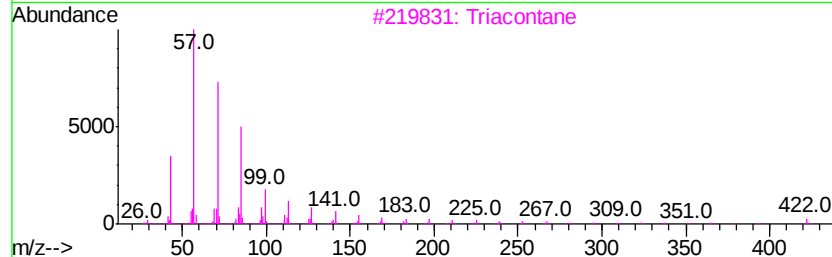
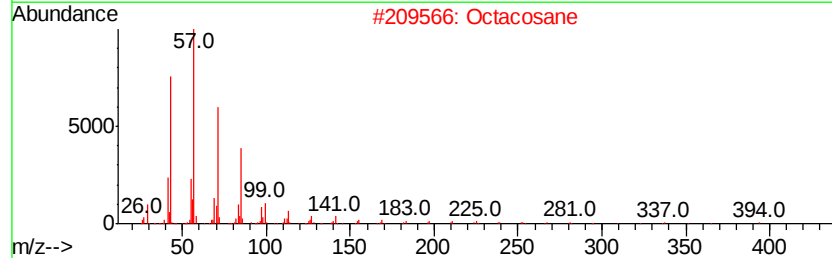
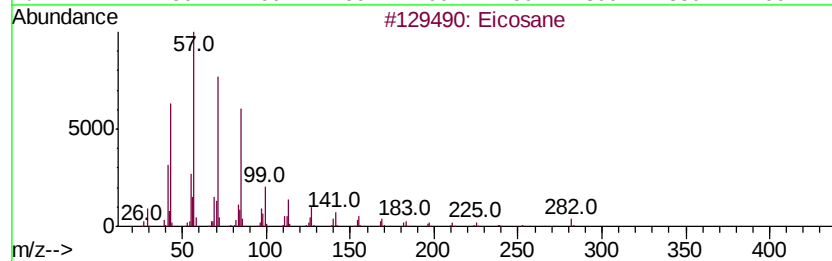
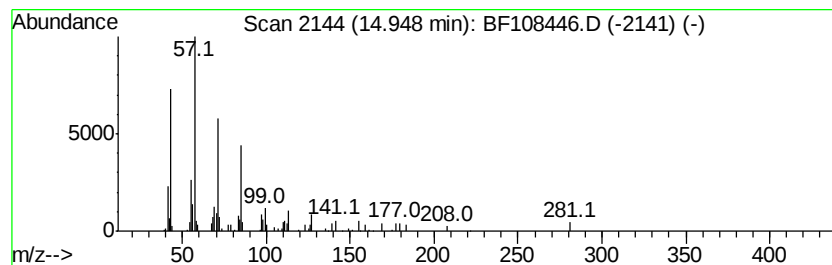
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.20 ng	86957	Chrysene-d12	14.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Octacosane	394	C28H58	000630-02-4	91
3		Triacotane	422	C30H62	000638-68-6	91
4		Octadecane	254	C18H38	000593-45-3	91
5		Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082318\
Data File : BF108446.D
Acq On : 24 Aug 2018 3:43
Operator : JU/SJ
Sample : J4546-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BRICK-WALL-BPM

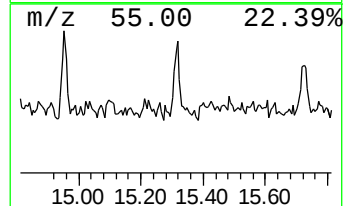
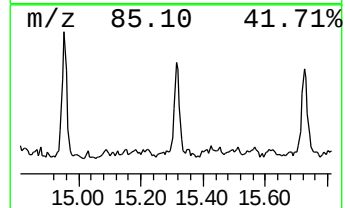
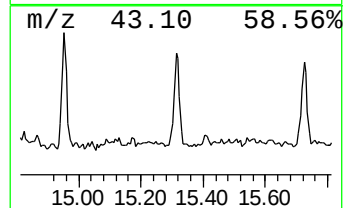
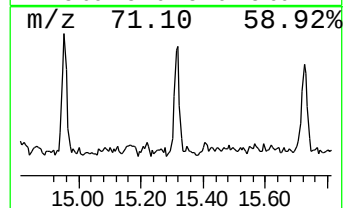
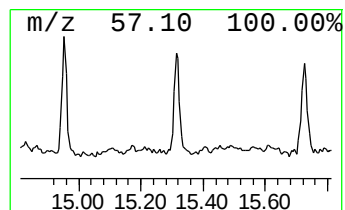
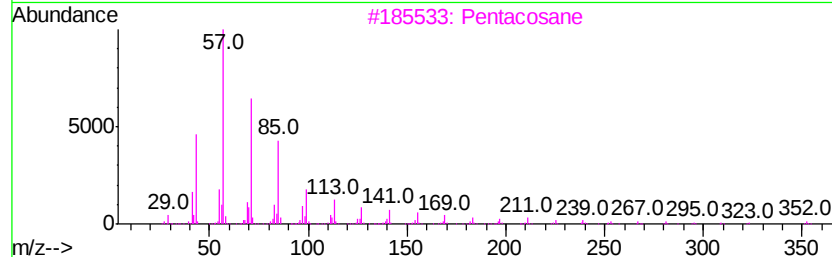
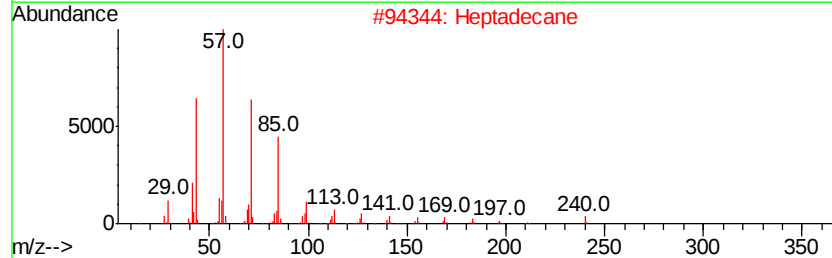
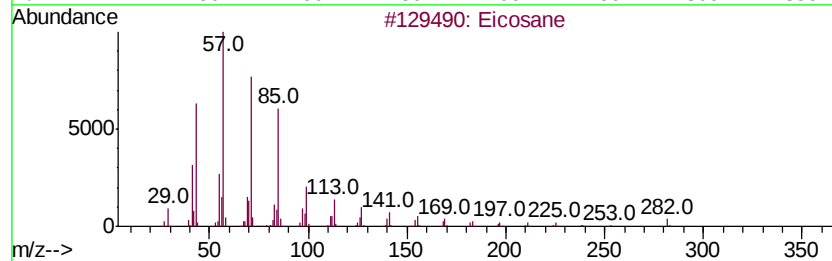
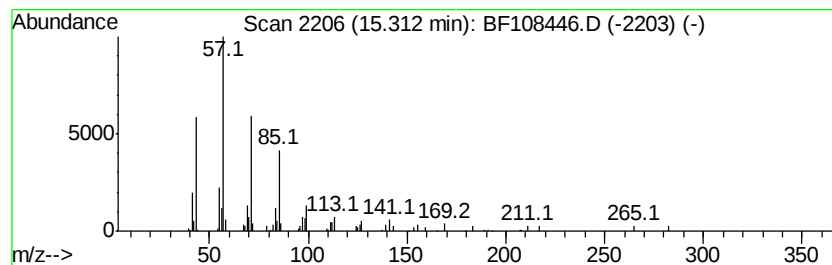
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	2.07 ng	78541	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	97
2		Heptadecane	240	C17H36	000629-78-7	91
3		Pentacosane	352	C25H52	000629-99-2	91
4		Octadecane	254	C18H38	000593-45-3	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082318\
Data File : BF108446.D
Acq On : 24 Aug 2018 3:43
Operator : JU/SJ
Sample : J4546-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BRICK-WALL-BPM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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
Butane, 2-methoxy...	2.38	10.8	ng	462435	1	7.00	853974	20.0
2-Pentanone, 4-hy...	5.25	3.1	ng	133794	1	7.00	853974	20.0
unknown6.77	6.77	76.6	ng	3269290	1	7.00	853974	20.0
Hexadecanoic acid...	12.92	3.5	ng	139427	5	14.19	790305	20.0
Octadecanoic acid...	13.63	2.1	ng	82483	5	14.19	790305	20.0
n-Tetracosanol-1	14.11	5.1	ng	201827	5	14.19	790305	20.0
Tridecane, 1-iodo-	14.62	2.1	ng	81360	5	14.19	790305	20.0
Eicosane	14.95	2.2	ng	86957	5	14.19	790305	20.0
Heptadecane	15.31	2.1	ng	78541	6	15.75	759535	20.0