

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102518\
 Data File : BF110160.D
 Acq On : 25 Oct 2018 14:33
 Operator : JU/SJ
 Sample : J5575-06
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SSSI-1015-S-DH-26

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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	2.346	38	44	52	rVB	494109	676605	14.30%	1.679%
2	3.616	258	260	271	rBV	26924	53217	1.12%	0.132%
3	5.222	529	533	545	rVB	151786	212865	4.50%	0.528%
4	5.598	591	597	600	rBV	3983339	4032192	85.22%	10.008%
5	6.593	760	766	771	rBV2	3608283	4623313	97.72%	11.476%
6	6.740	785	791	794	rBV	4296891	4290835	90.69%	10.650%
7	6.963	826	829	833	rBV	1083839	938550	19.84%	2.330%
8	7.122	852	856	860	rBV	3499486	3295971	69.66%	8.181%
9	7.534	919	926	929	rBV	2477527	2779221	58.74%	6.898%
10	8.251	1043	1048	1051	rBV	1290013	1198547	25.33%	2.975%
11	9.328	1225	1231	1234	rBV	4867204	4731266	100.00%	11.744%
12	9.716	1293	1297	1301	rBV	481984	437204	9.24%	1.085%
13	10.010	1342	1347	1355	rVB	1547484	1369151	28.94%	3.398%
14	10.804	1477	1482	1485	rBV	2966566	2830934	59.83%	7.027%
15	11.498	1597	1600	1604	rBV	1411213	1288820	27.24%	3.199%
16	12.010	1683	1687	1699	rBV2	129729	154456	3.26%	0.383%
17	13.086	1865	1870	1873	rBV	3742156	3637043	76.87%	9.028%
18	13.969	2016	2020	2032	rVB	205441	266920	5.64%	0.663%
19	14.145	2046	2050	2054	rBV	893724	786679	16.63%	1.953%
20	14.286	2070	2074	2079	rBV	82915	74702	1.58%	0.185%
21	14.592	2122	2126	2131	rBV	163221	157183	3.32%	0.390%
22	14.916	2175	2181	2187	rBV	227340	271586	5.74%	0.674%
23	15.268	2236	2241	2250	rVB	297185	367804	7.77%	0.913%
24	15.674	2303	2310	2315	rBV2	816895	1150050	24.31%	2.855%
25	16.133	2381	2388	2395	rBV	236523	381906	8.07%	0.948%
26	16.668	2473	2479	2488	rVB	110050	210213	4.44%	0.522%
27	17.298	2581	2586	2594	rVB3	33992	70561	1.49%	0.175%

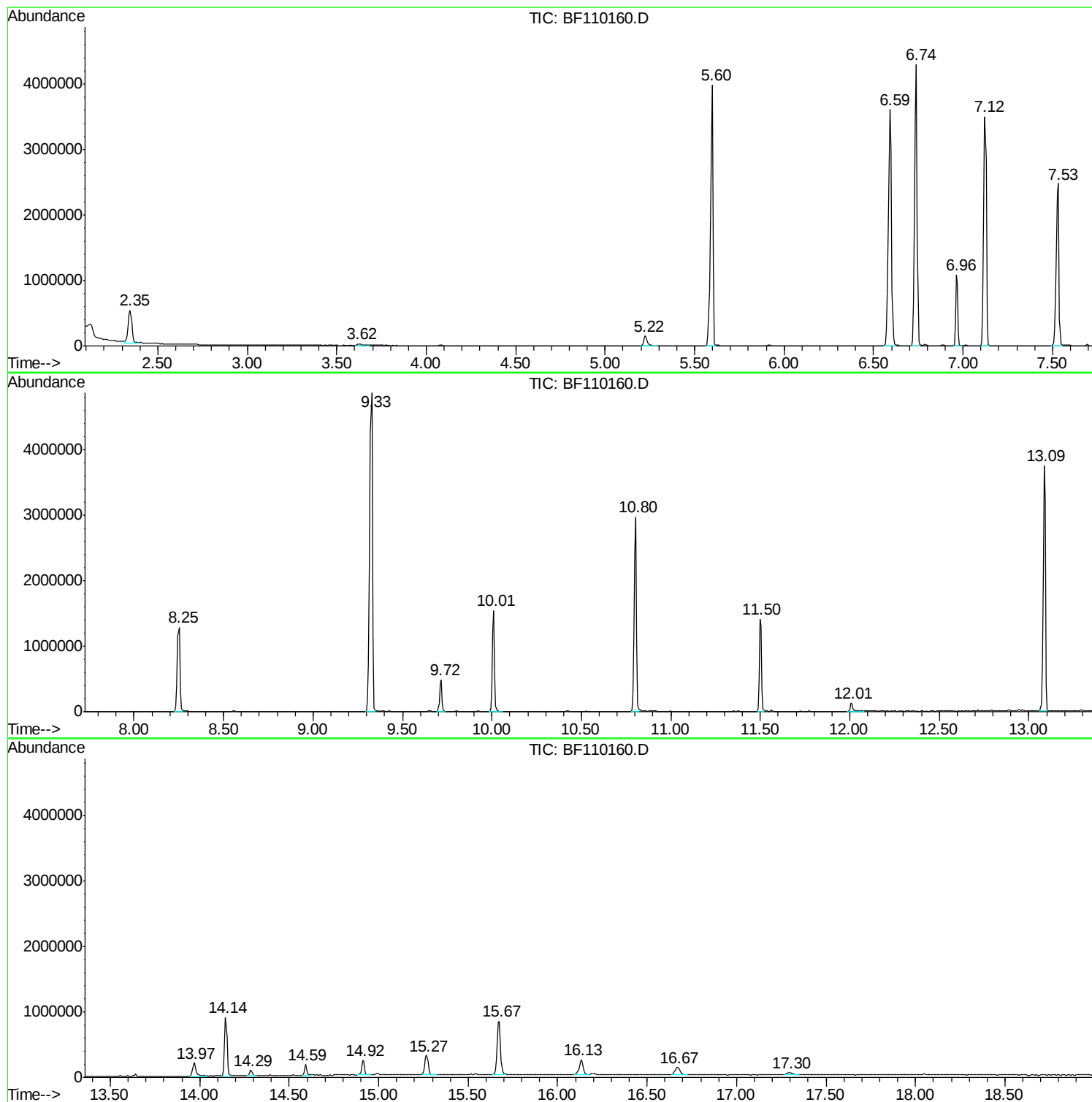
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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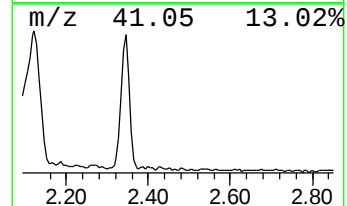
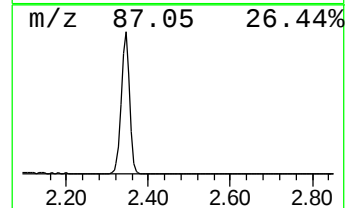
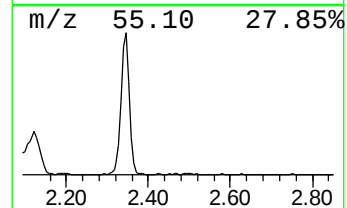
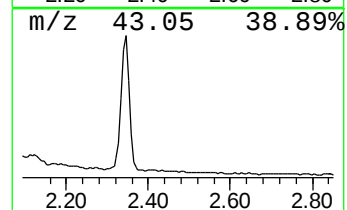
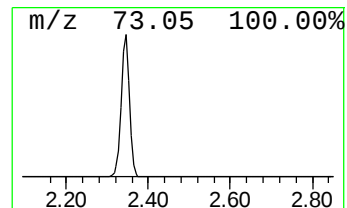
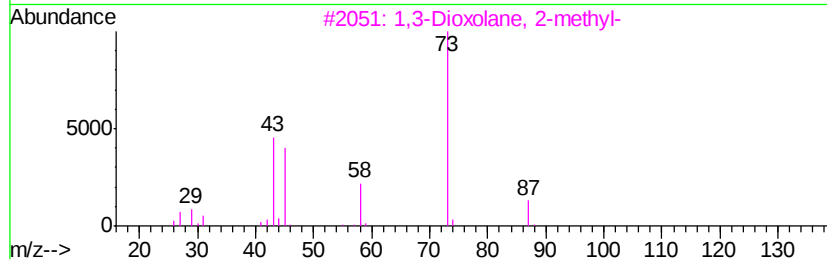
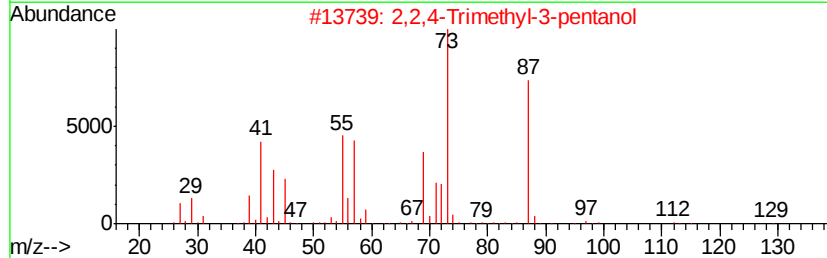
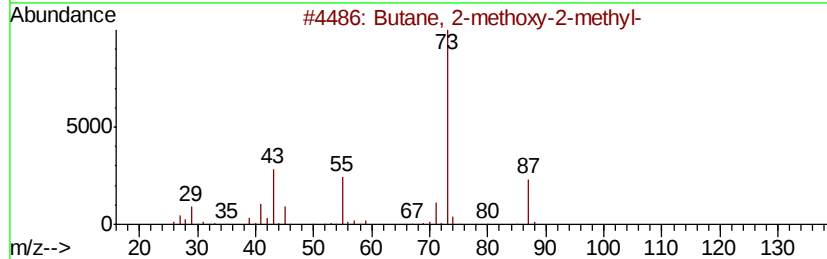
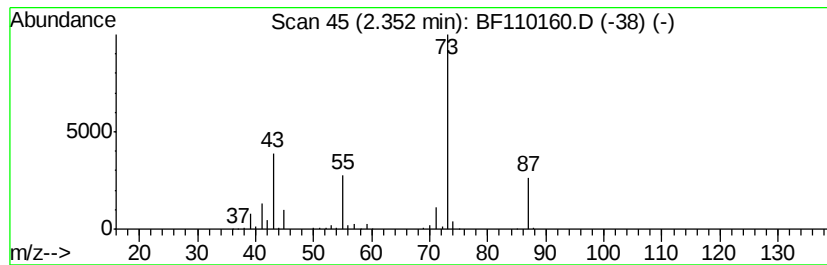
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.35	14.42 ng	676605	1,4-Dichlorobenzene-d4	6.96

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		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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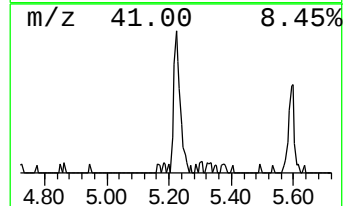
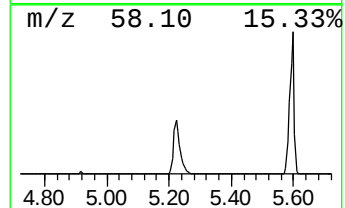
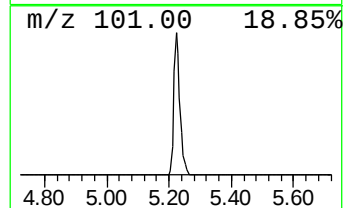
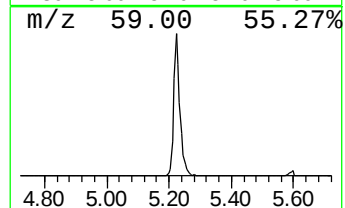
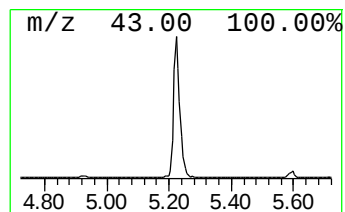
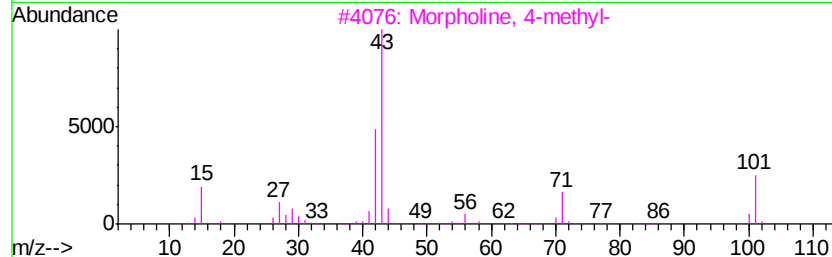
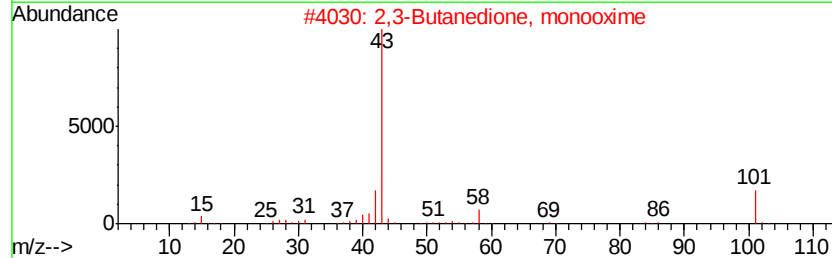
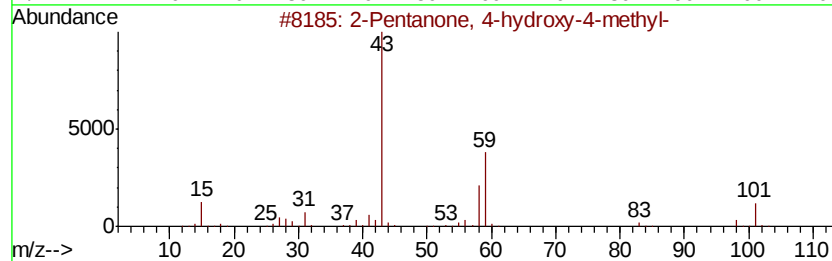
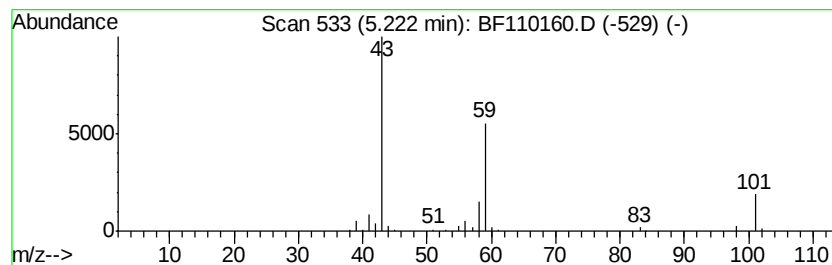
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	4.54 ng	212865	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		1,2-Butanediol	90	C4H10O2	000584-03-2	9



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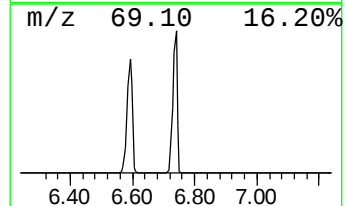
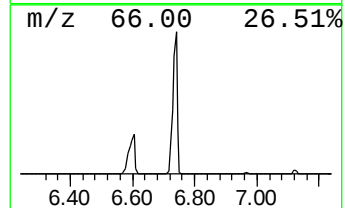
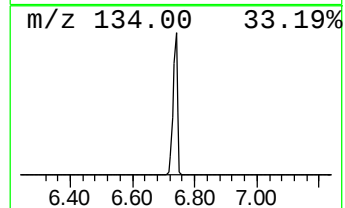
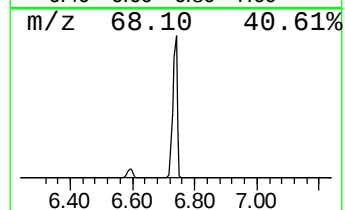
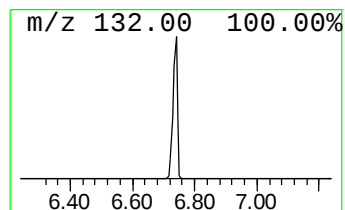
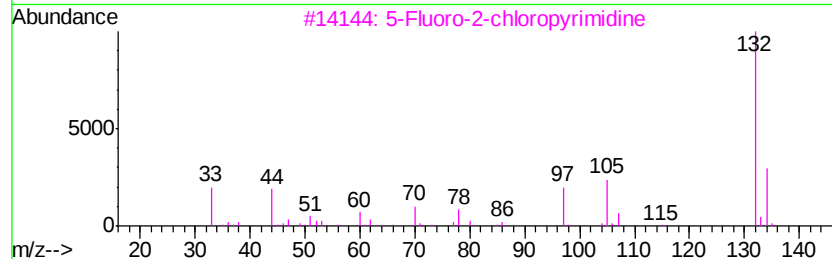
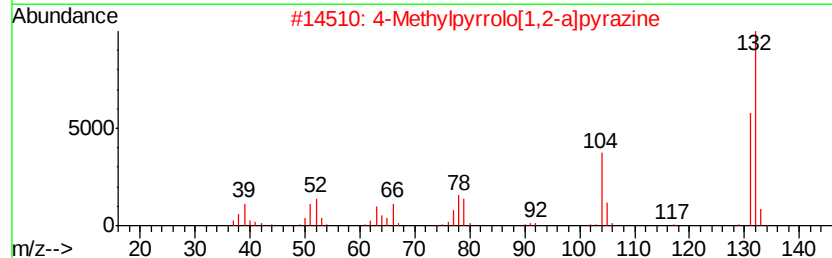
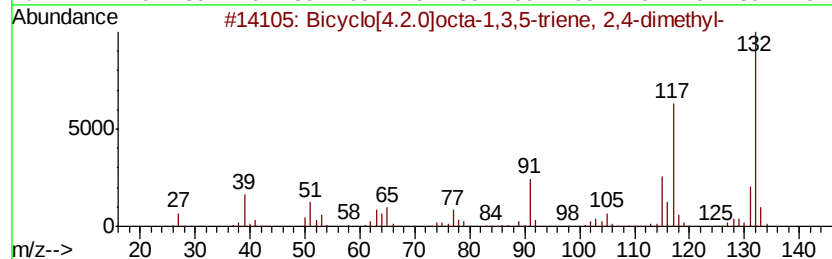
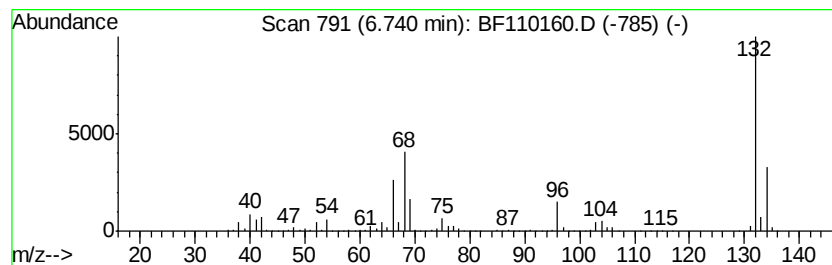
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Peak Number 3 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	91.44 ng	4290840	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
2		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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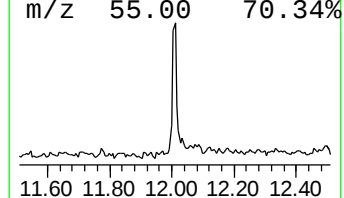
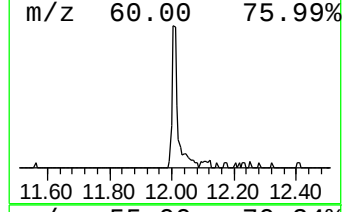
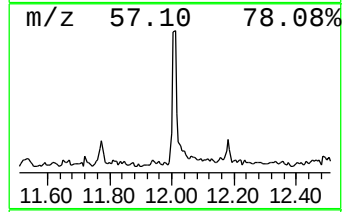
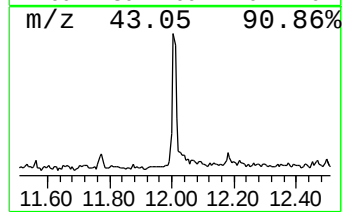
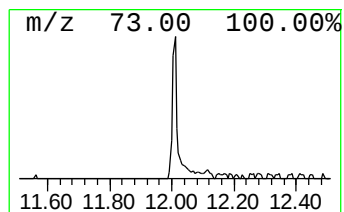
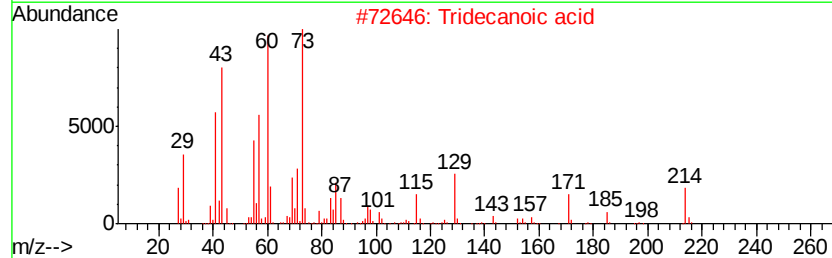
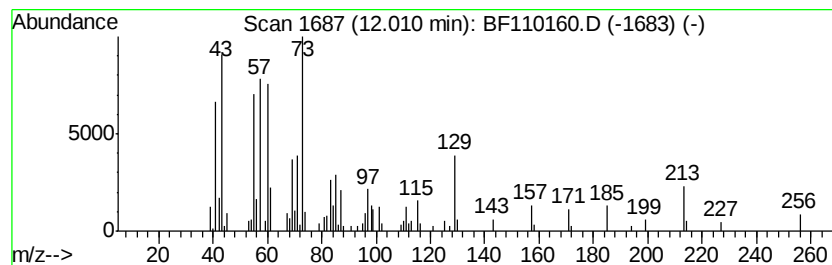
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.40 ng	154456	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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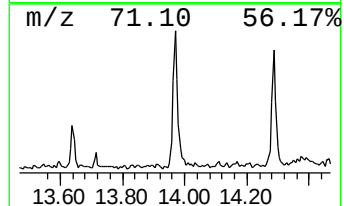
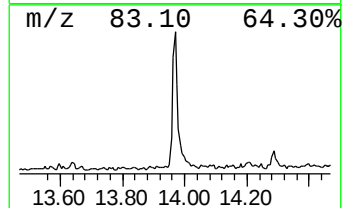
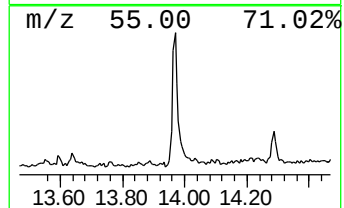
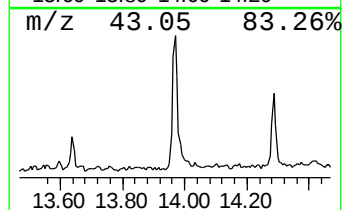
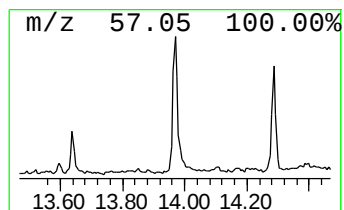
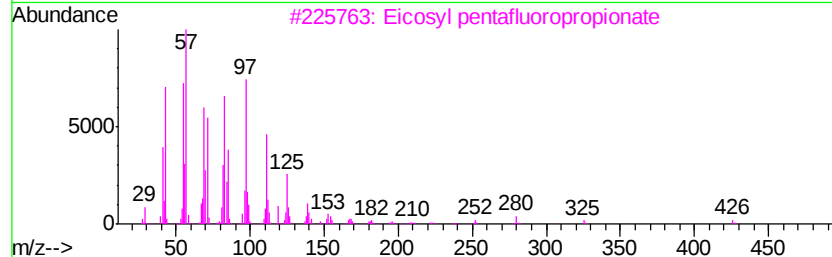
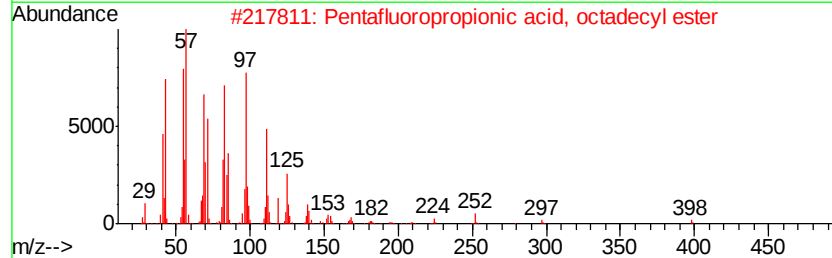
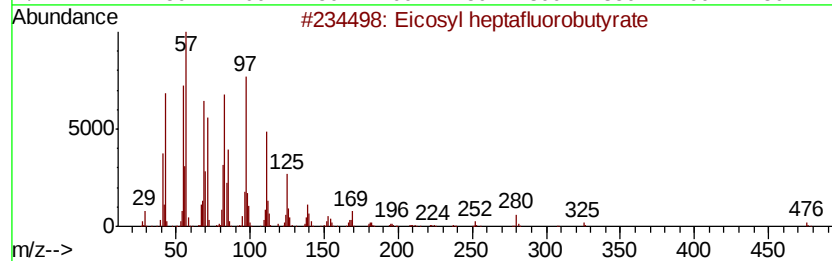
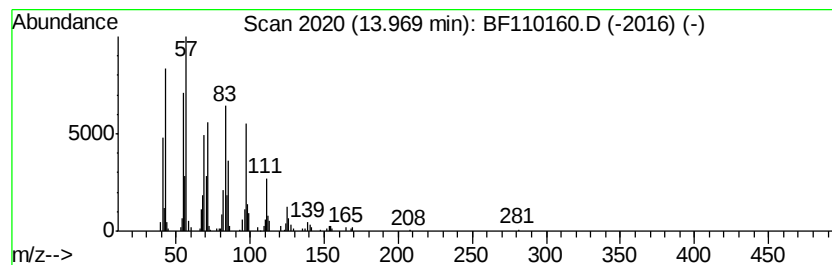
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Peak Number 6 Eicosyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.97	6.79 ng	266920	Chrysene-d12		14.15	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosyl	heptafluorobutvrate	494	C24H41F7O2	1000351-83-5	91
2	Pentafluoropropionic acid,	octad...	416	C21H37F5O2	959261-25-7	91
3	Eicosyl	pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
4	Heptafluorobutyric acid,	n-octad...	466	C22H37F7O2	000400-57-7	91
5	1-Hexadecanesulfonyl	chloride	324	C16H33ClO2S	038775-38-1	91



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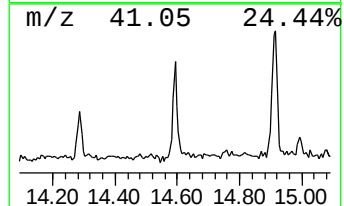
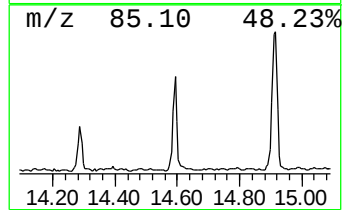
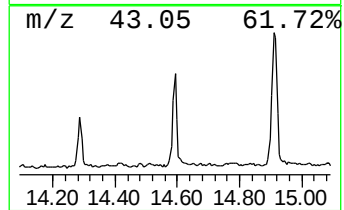
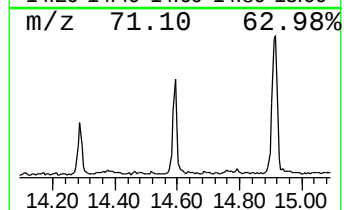
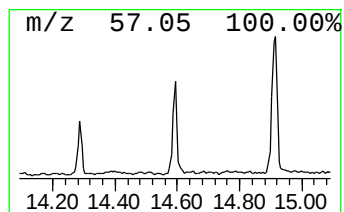
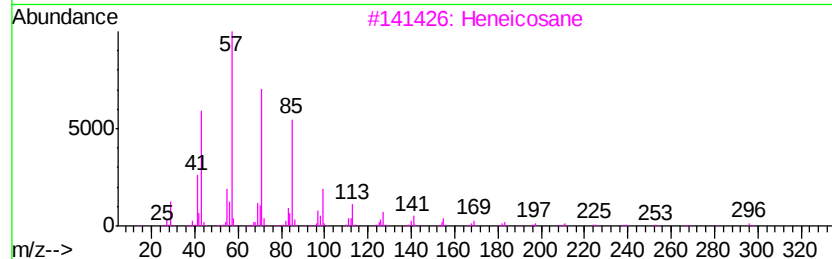
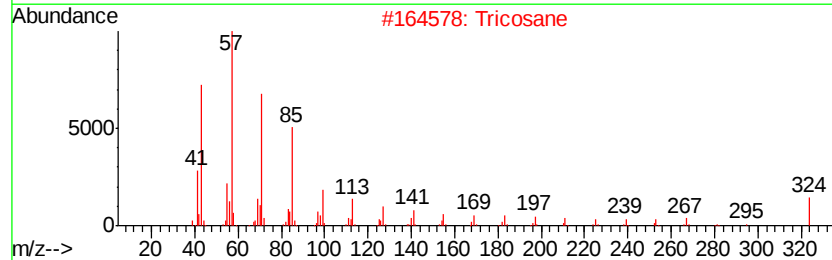
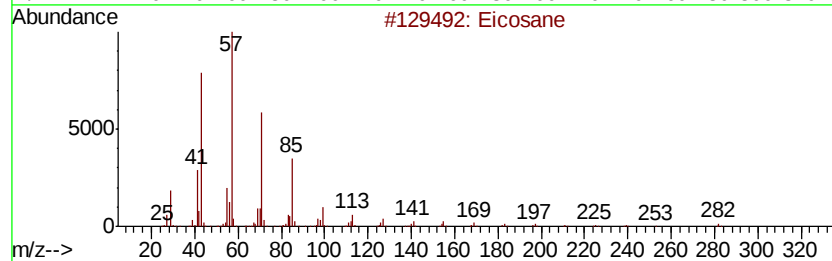
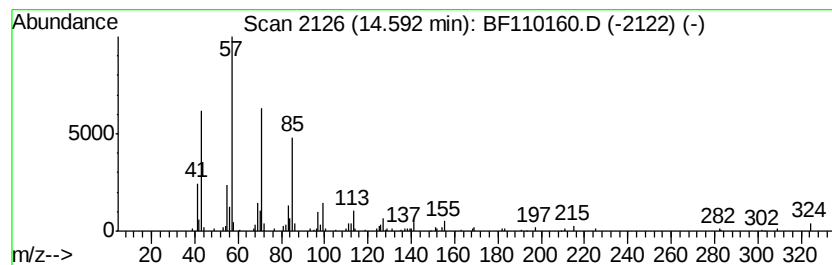
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	4.00 ng	157183	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Tricosane	324	C23H48	000638-67-5	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Hexacosane	366	C26H54	000630-01-3	90
5		Tetracosane	338	C24H50	000646-31-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110160.D
Acq On : 25 Oct 2018 14:33
Operator : JU/SJ
Sample : J5575-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SSSI-1015-S-DH-26

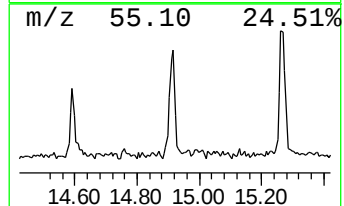
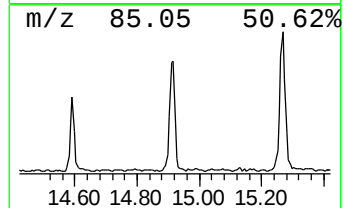
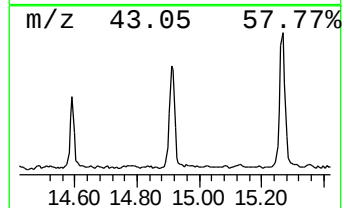
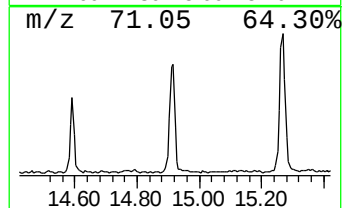
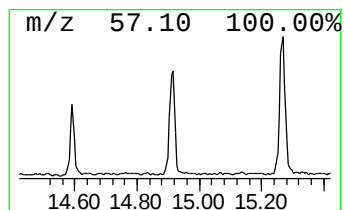
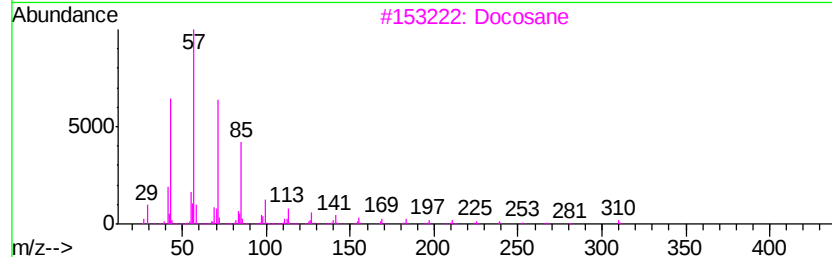
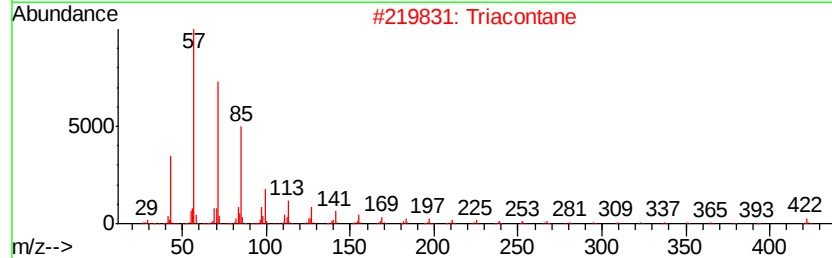
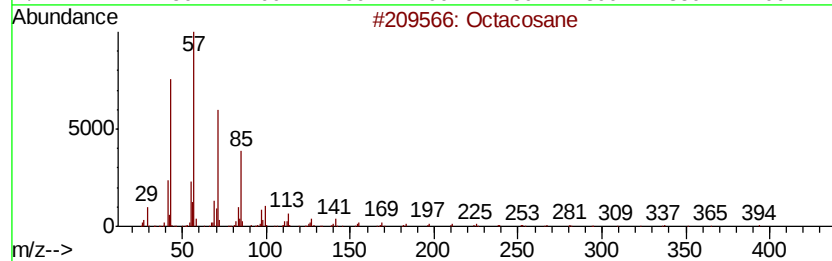
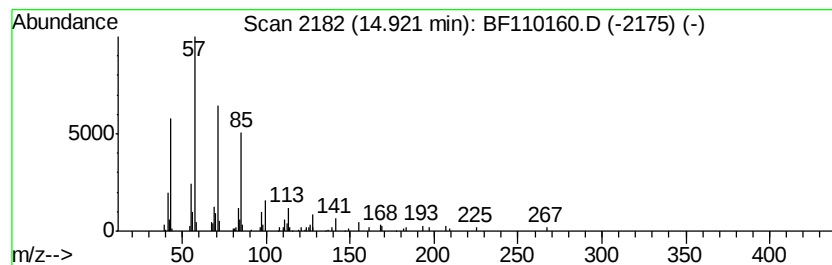
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	4.72 ng	271586	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Triacontane	422	C30H62	000638-68-6	91
3		Docosane	310	C22H46	000629-97-0	91
4		Heneicosane	296	C21H44	000629-94-7	90
5		Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110160.D
Acq On : 25 Oct 2018 14:33
Operator : JU/SJ
Sample : J5575-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SSSI-1015-S-DH-26

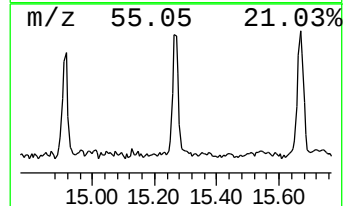
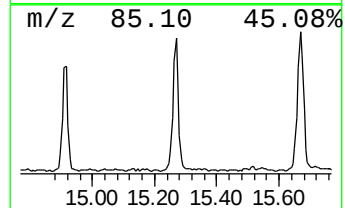
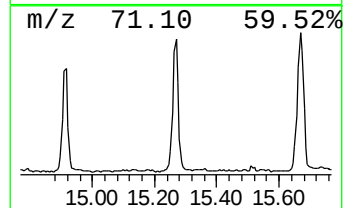
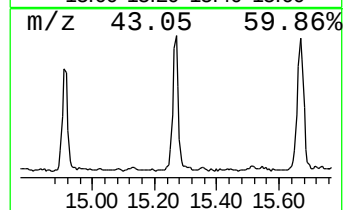
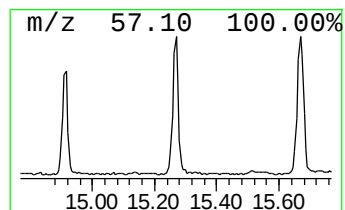
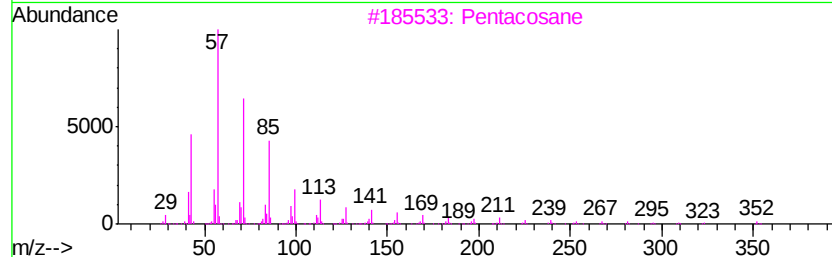
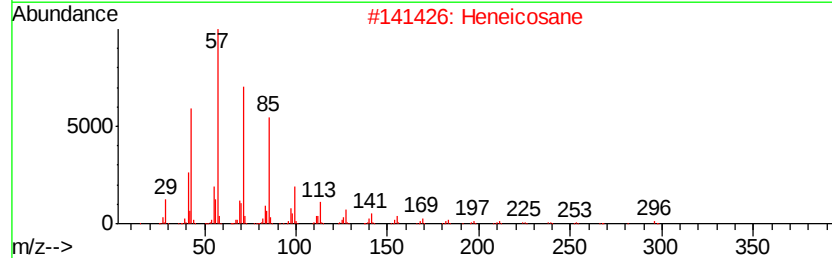
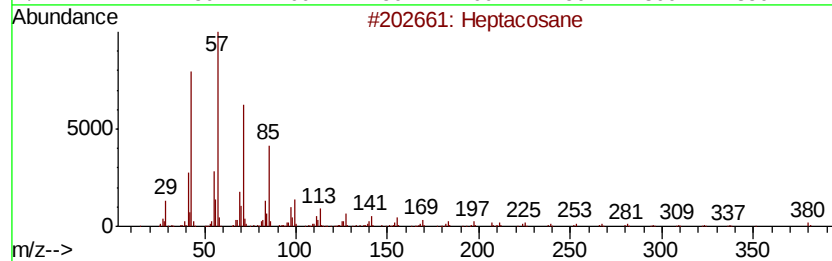
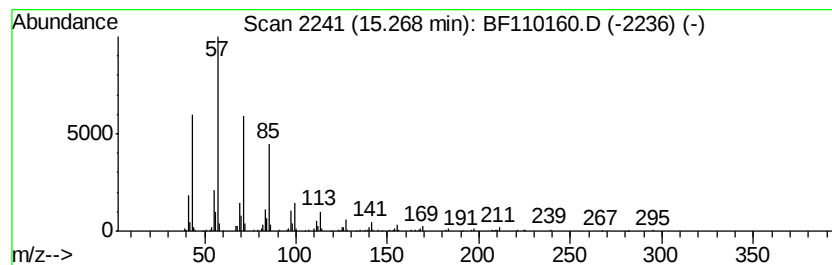
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	6.40 ng	367804	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Pentacosane	352	C25H52	000629-99-2	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110160.D
Acq On : 25 Oct 2018 14:33
Operator : JU/SJ
Sample : J5575-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SSSI-1015-S-DH-26

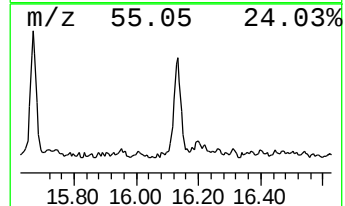
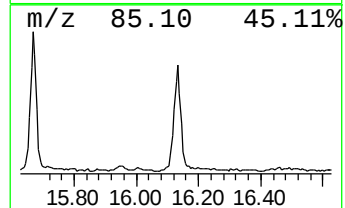
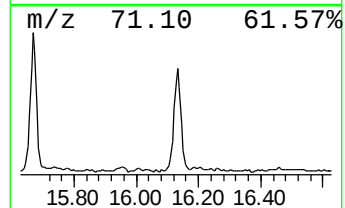
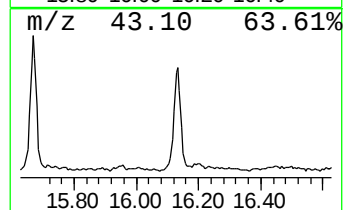
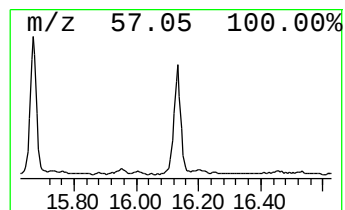
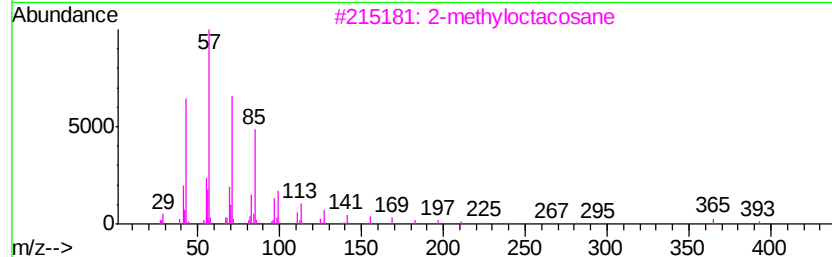
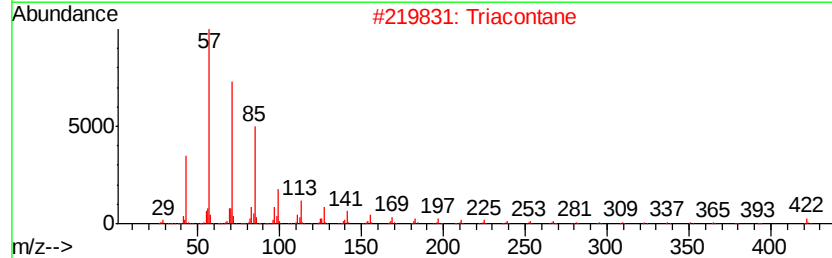
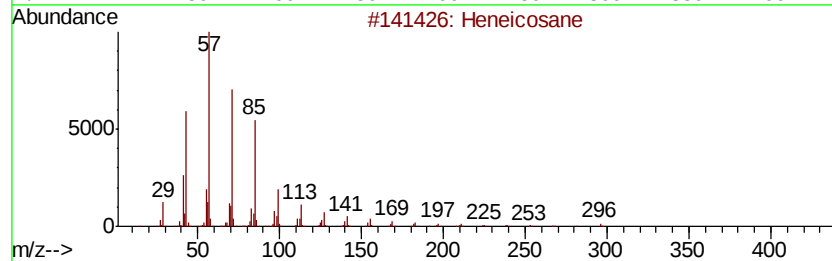
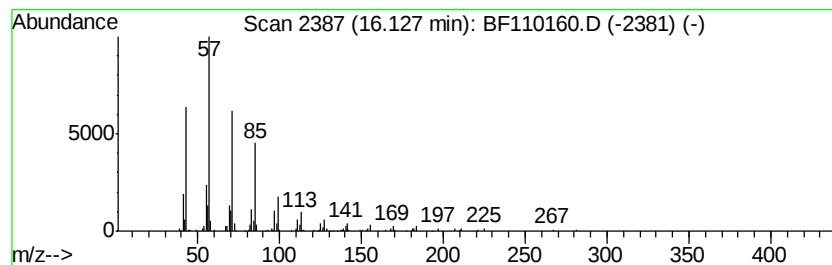
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	6.64 ng	381906	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Triacontane	422	C30H62	000638-68-6	91
3			2-methyloctacosane	408	C29H60	1000376-72-8	90
4			Octacosane	394	C28H58	000630-02-4	90
5			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102518\
Data File : BF110160.D
Acq On : 25 Oct 2018 14:33
Operator : JU/SJ
Sample : J5575-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SSSI-1015-S-DH-26

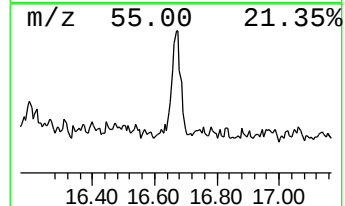
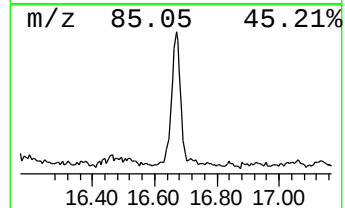
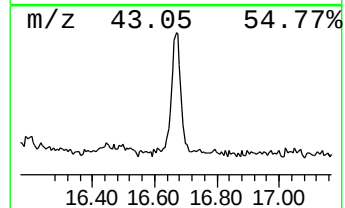
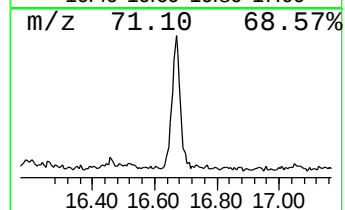
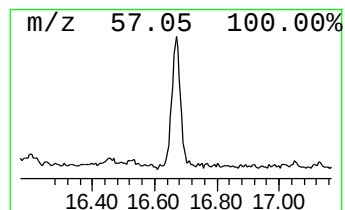
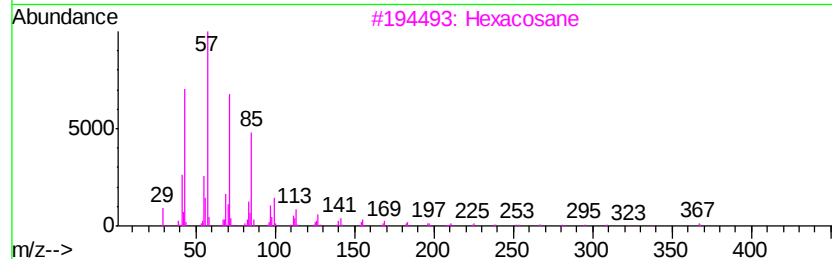
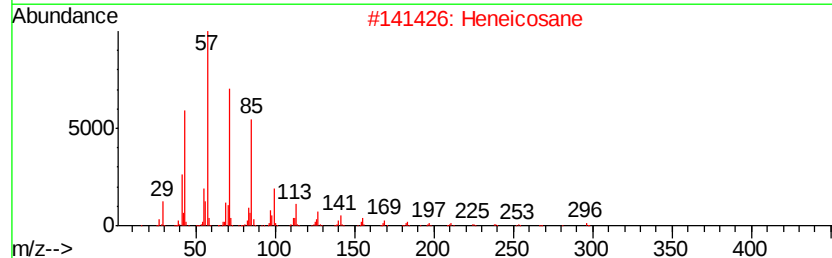
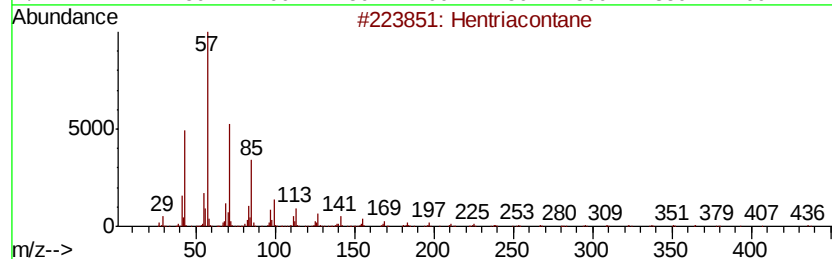
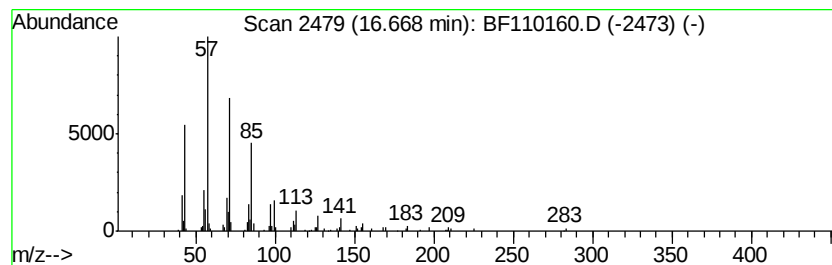
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hentriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.67	3.66 ng	210213	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102518\
Data File : BF110160.D
Acq On : 25 Oct 2018 14:33
Operator : JU/SJ
Sample : J5575-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SSSI-1015-S-DH-26

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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2-Pentanone, 4-hy...	5.22	4.5	ng	212865	1	6.96	938550	20.0
unknown6.74	6.74	91.4	ng	4290840	1	6.96	938550	20.0
n-Hexadecanoic acid	12.01	2.4	ng	154456	4	11.50	1288820	20.0
Eicosyl heptaflu...	13.97	6.8	ng	266920	5	14.15	786679	20.0
Eicosane	14.59	4.0	ng	157183	5	14.15	786679	20.0
Octacosane	14.92	4.7	ng	271586	6	15.67	1150050	20.0
Heptacosane	15.27	6.4	ng	367804	6	15.67	1150050	20.0
Heneicosane	16.13	6.6	ng	381906	6	15.67	1150050	20.0
Hentriacontane	16.67	3.7	ng	210213	6	15.67	1150050	20.0