

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
 Data File : BF109938.D
 Acq On : 17 Oct 2018 23:29
 Operator : JU/SJ
 Sample : J5539-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-6-0.3-2FT

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-BF101518.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	2.322	35	40	48	rVB	593201	782528	16.31%	1.728%
2	5.216	528	532	540	rVB	181684	211812	4.41%	0.468%
3	5.598	592	597	600	rBV	4745817	4485385	93.49%	9.905%
4	6.592	760	766	771	rBV	4400850	4797557	100.00%	10.594%
5	6.745	787	792	795	rBV	5033541	4624570	96.39%	10.212%
6	6.975	827	831	835	rBV	1759760	1438145	29.98%	3.176%
7	7.133	854	858	861	rBV	4255281	3584582	74.72%	7.916%
8	7.539	921	927	930	rBV	3021870	2877280	59.97%	6.354%
9	8.257	1045	1049	1053	rBV	1965117	1767978	36.85%	3.904%
10	9.333	1227	1232	1235	rBV	5484089	4517890	94.17%	9.977%
11	9.722	1295	1298	1301	rBV	601198	433439	9.03%	0.957%
12	10.016	1345	1348	1352	rBV	1896294	1712599	35.70%	3.782%
13	10.804	1478	1482	1486	rBV	2410346	2326326	48.49%	5.137%
14	11.510	1598	1602	1605	rBV	1779759	1467269	30.58%	3.240%
15	12.015	1684	1688	1693	rBV	85905	81513	1.70%	0.180%
16	13.092	1867	1871	1875	rBV	3853201	3429069	71.48%	7.572%
17	13.562	1946	1951	1956	rBV2	49142	54820	1.14%	0.121%
18	13.651	1962	1966	1969	rBV2	60513	59252	1.24%	0.131%
19	13.974	2017	2021	2033	rBV	336584	392800	8.19%	0.867%
20	14.151	2047	2051	2055	rBV	1606131	1546481	32.23%	3.415%
21	14.298	2072	2076	2079	rBV	165752	139271	2.90%	0.308%
22	14.604	2124	2128	2134	rBV	258002	252163	5.26%	0.557%
23	14.927	2177	2183	2188	rBV	363201	401400	8.37%	0.886%
24	15.009	2193	2197	2202	rVB	148945	160673	3.35%	0.355%
25	15.286	2239	2244	2253	rBV	398860	506955	10.57%	1.119%
26	15.680	2305	2311	2321	rBV2	1498920	2094147	43.65%	4.624%
27	16.150	2386	2391	2397	rBV	315607	488860	10.19%	1.080%
28	16.203	2397	2400	2406	rVB2	41277	64844	1.35%	0.143%
29	16.698	2477	2484	2489	rBV	186937	358996	7.48%	0.793%
30	17.333	2586	2592	2600	rVB	74668	146783	3.06%	0.324%
31	17.862	2678	2682	2691	rVB10	38657	79109	1.65%	0.175%

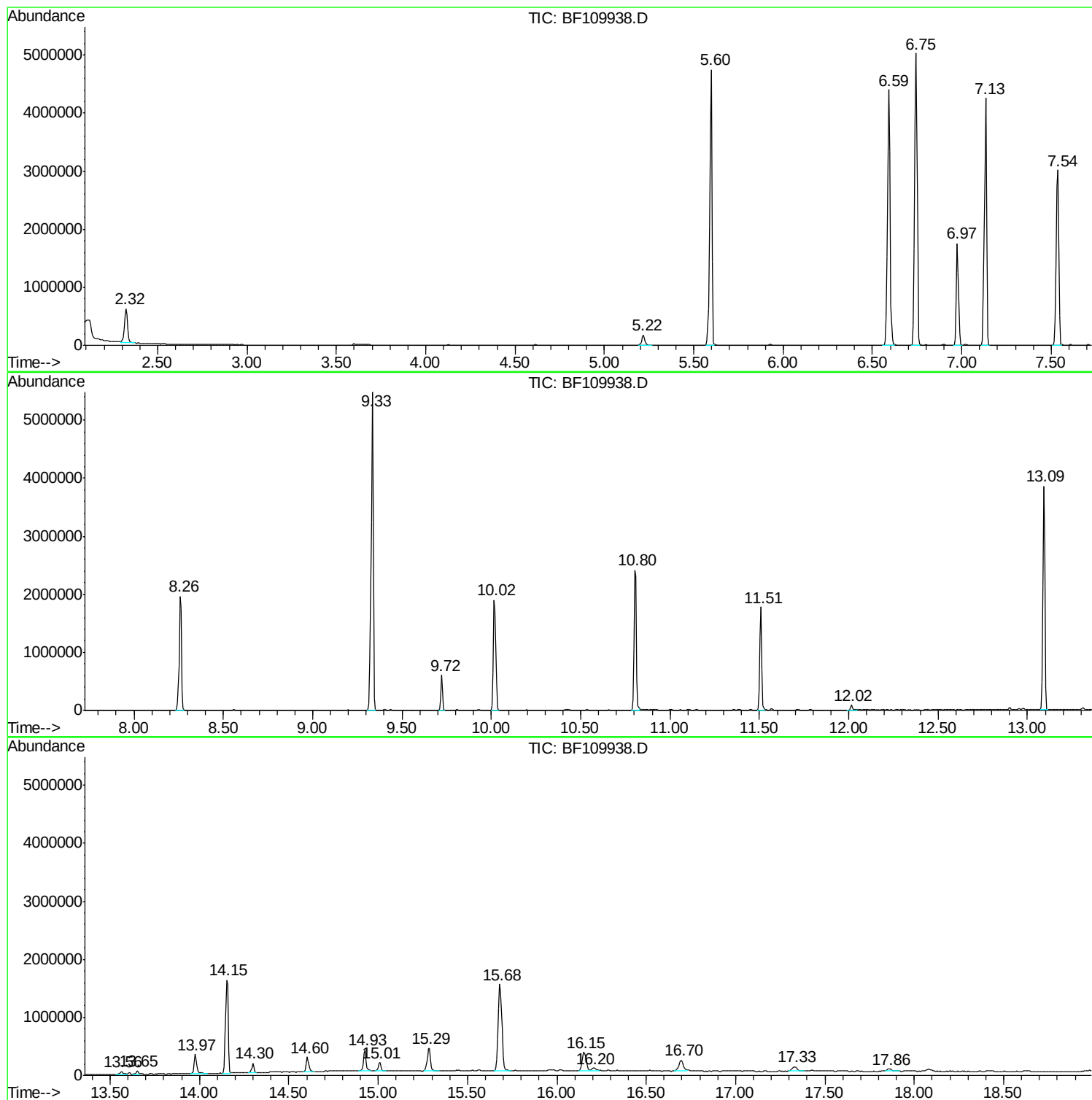
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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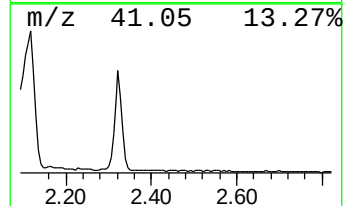
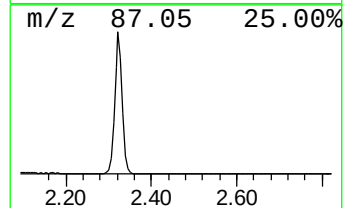
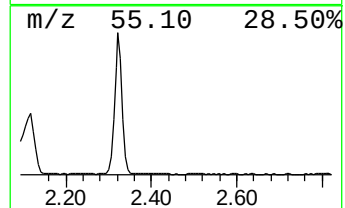
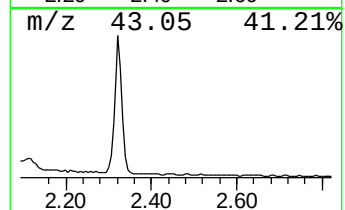
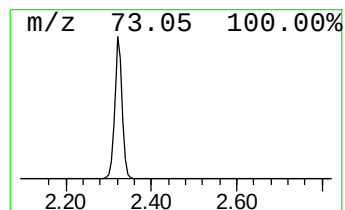
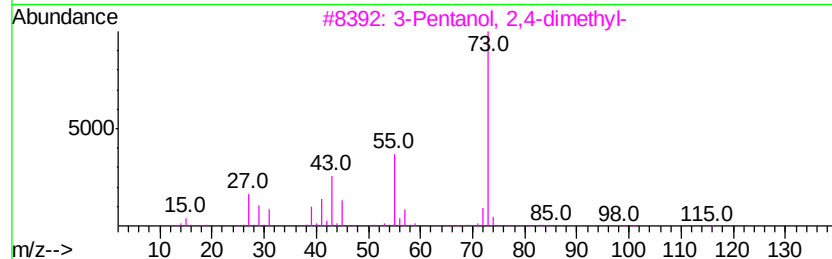
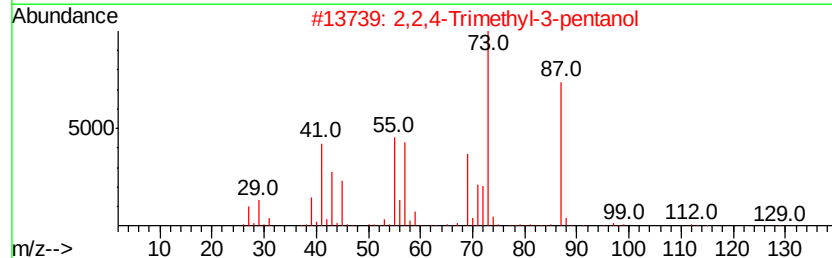
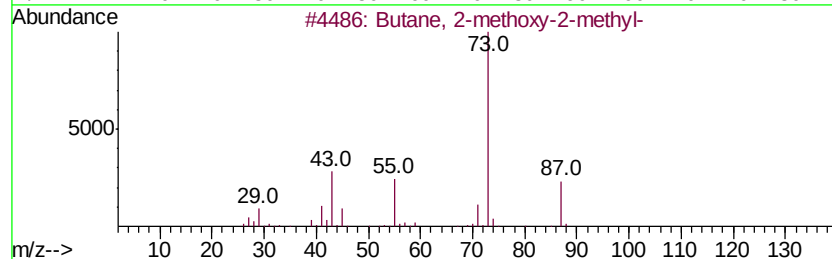
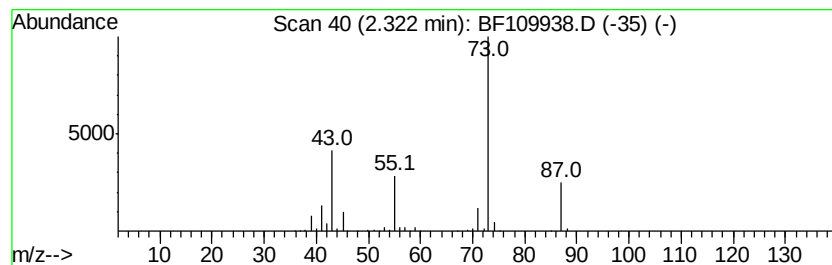
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.32	10.88 ng	782528	1,4-Dichlorobenzene-d4	6.97

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		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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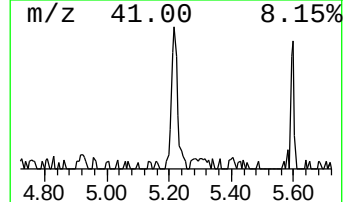
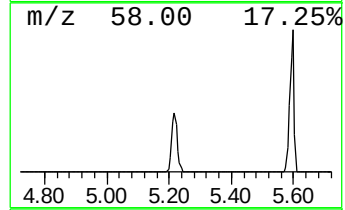
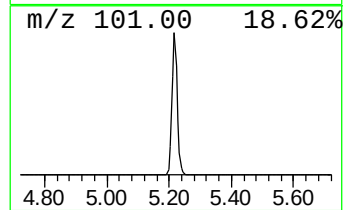
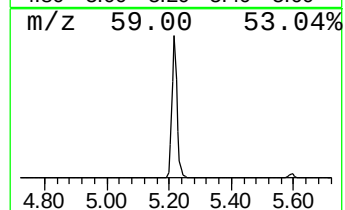
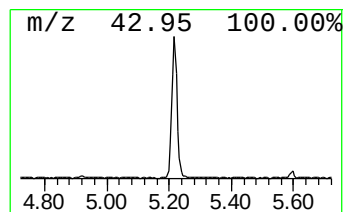
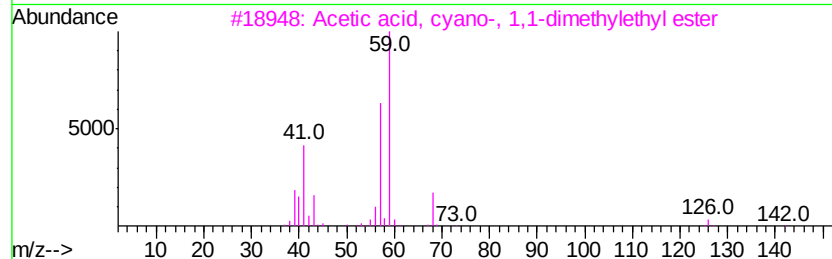
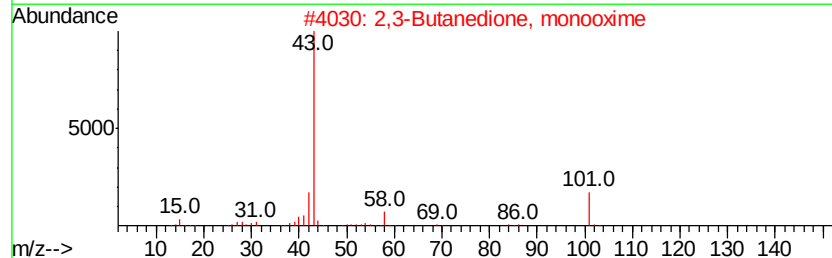
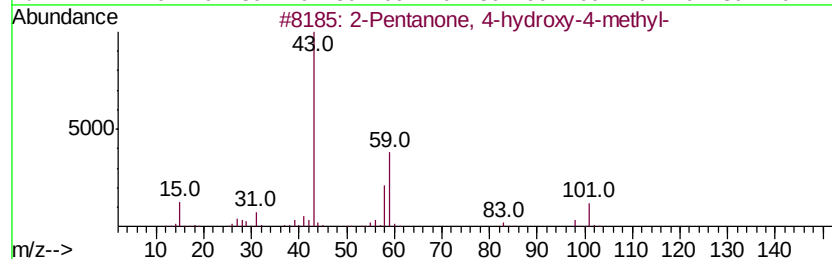
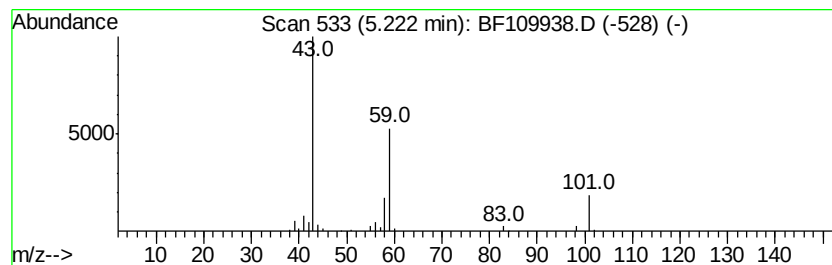
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	2.95 ng	211812	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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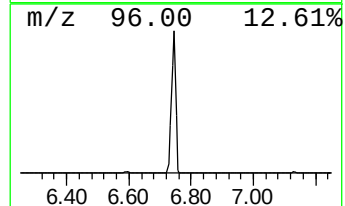
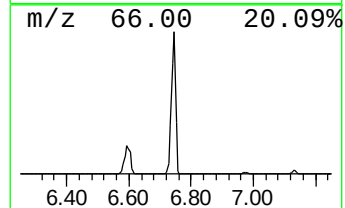
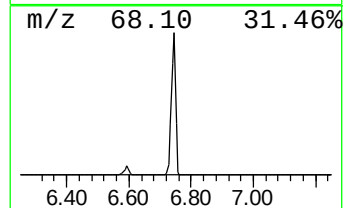
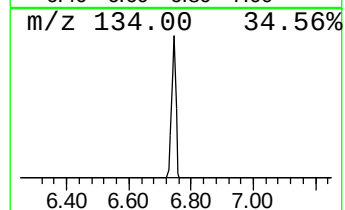
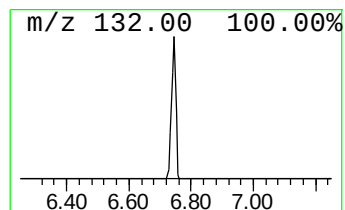
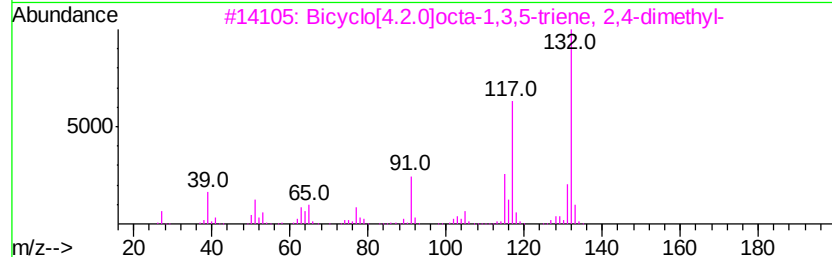
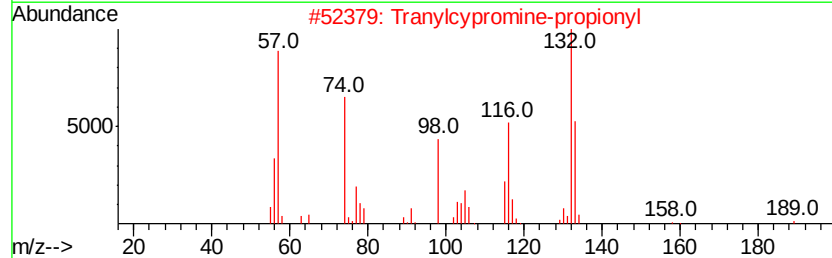
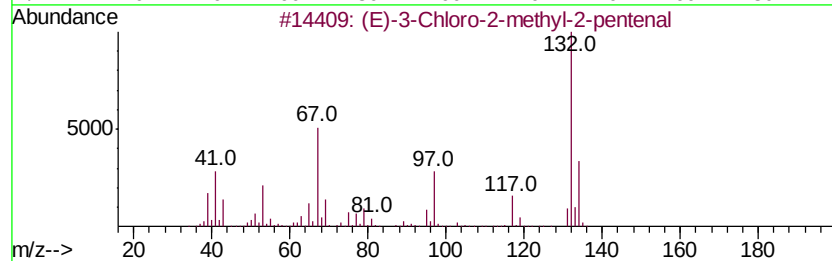
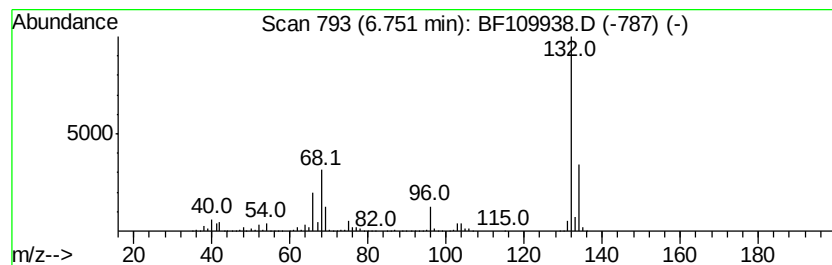
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	64.31 ng	4624570	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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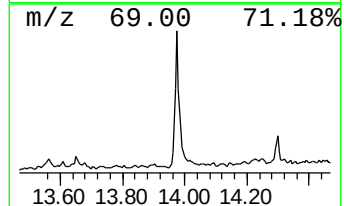
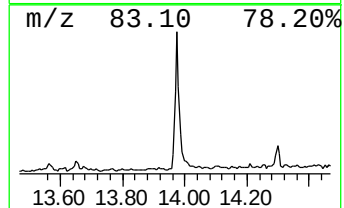
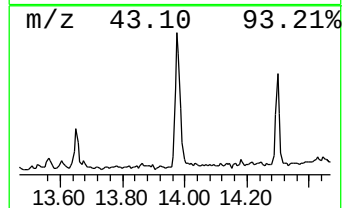
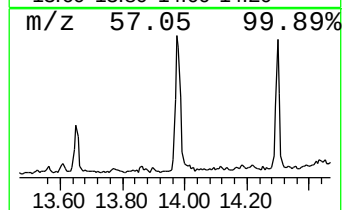
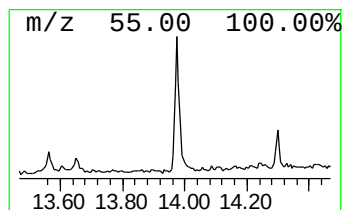
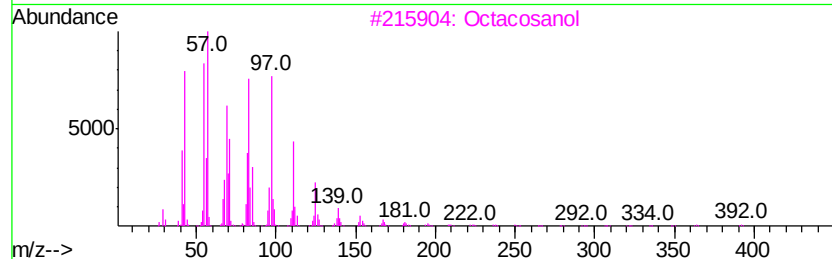
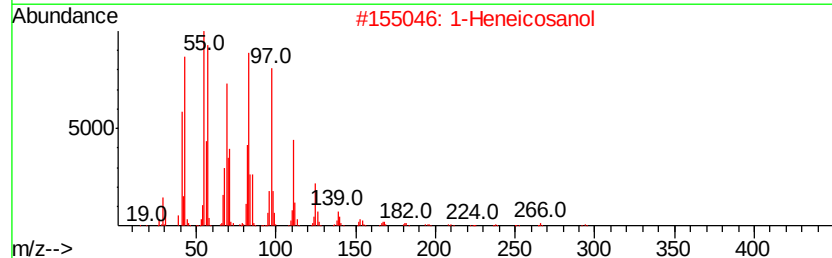
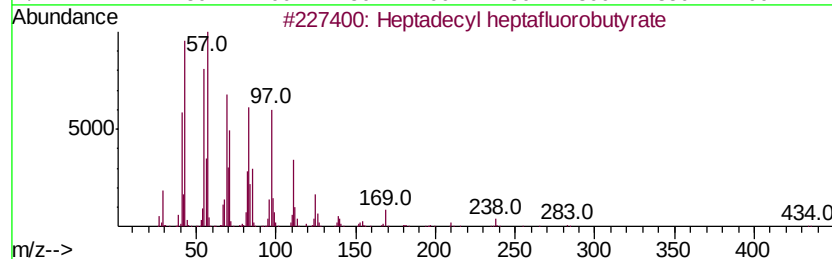
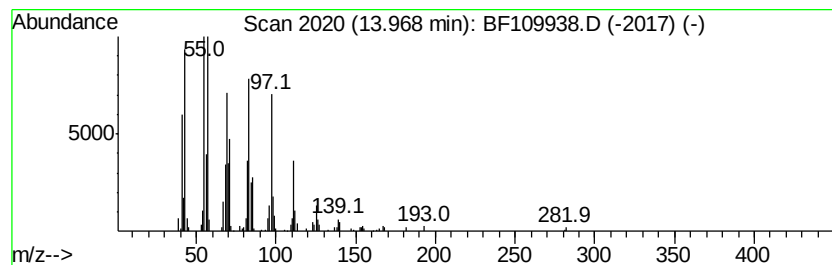
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Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	5.08 ng	392800	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		Octacosanol	410	C28H58O	000557-61-9	91
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91



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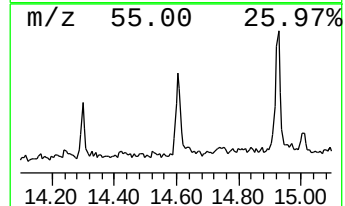
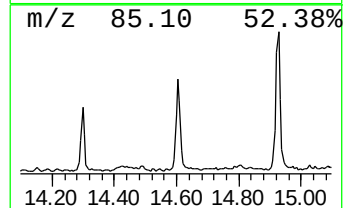
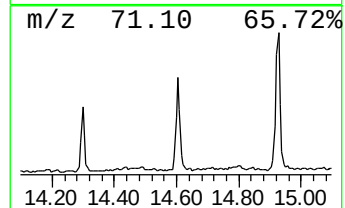
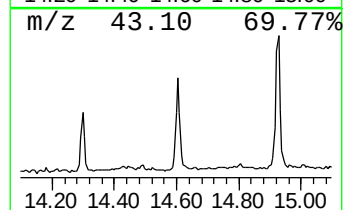
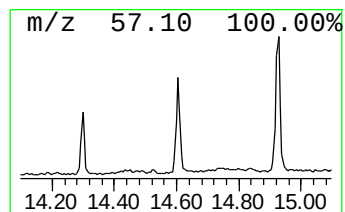
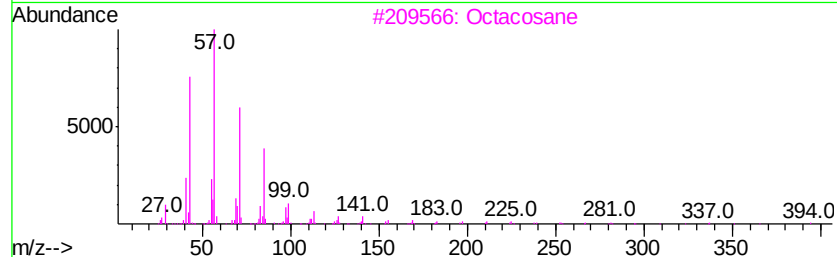
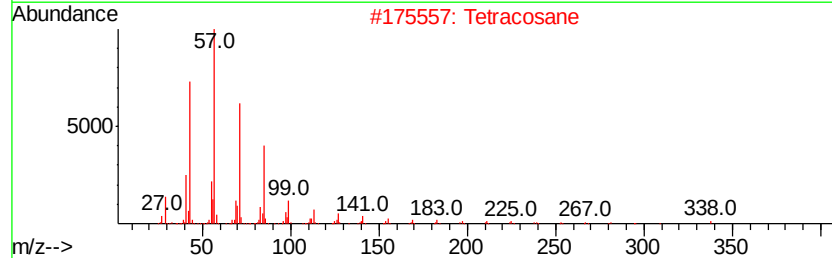
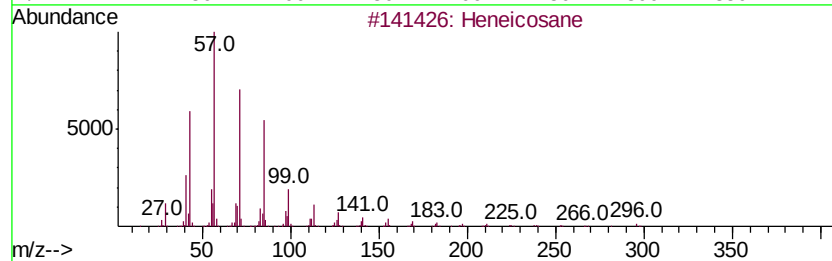
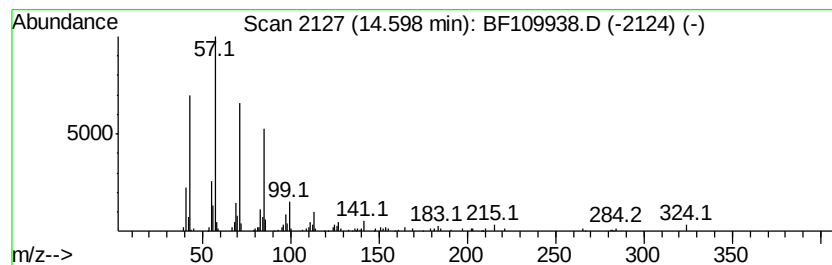
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	3.26 ng	252163	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Tetracosane		338	C24H50	000646-31-1	90
3	Octacosane		394	C28H58	000630-02-4	90
4	Hexacosane		366	C26H54	000630-01-3	90
5	Tricosane		324	C23H48	000638-67-5	90



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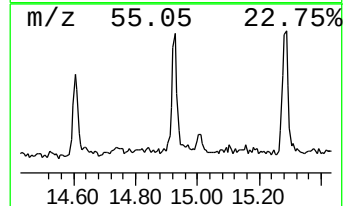
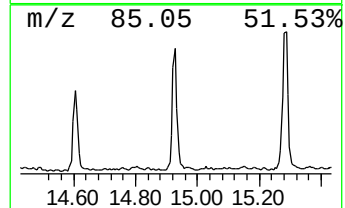
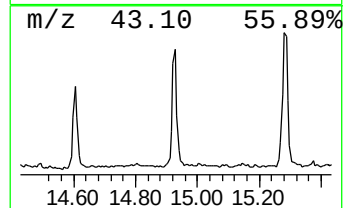
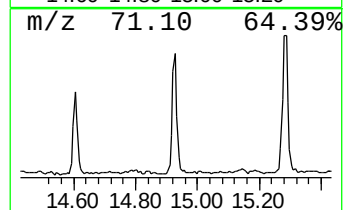
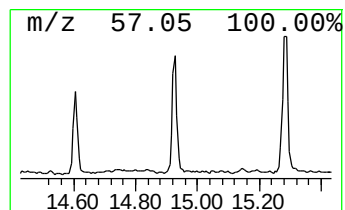
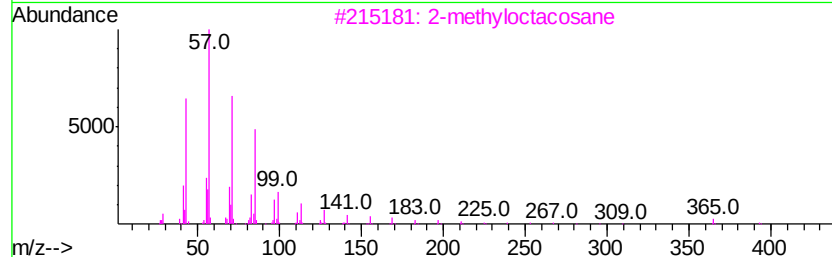
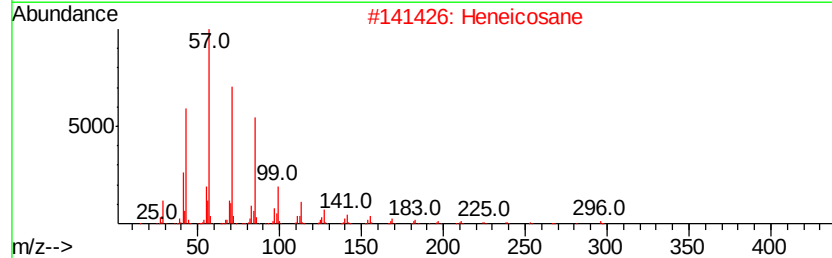
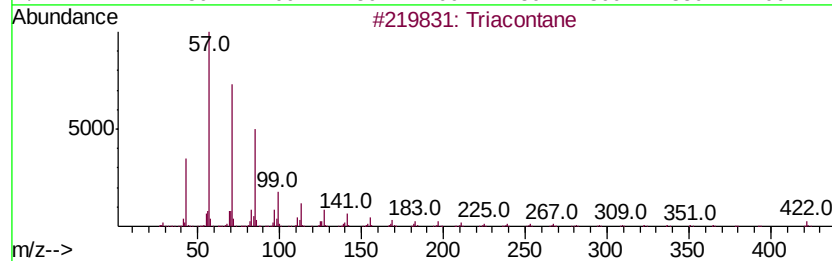
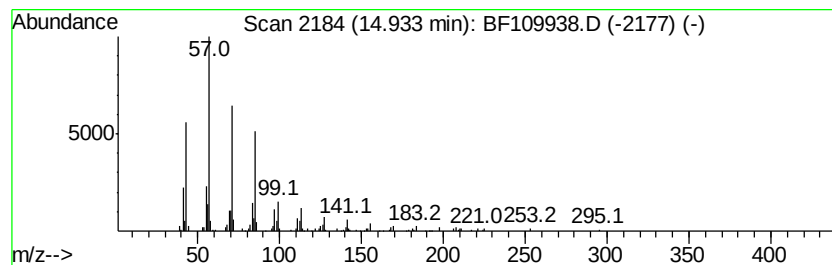
Instrument :
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ClientSampleId :
SB-6-0.3-2FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.93	3.83 ng	401400	Perylene-d12	15.68	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	Hexadecane	226	C16H34	000544-76-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109938.D
Acq On : 17 Oct 2018 23:29
Operator : JU/SJ
Sample : J5539-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-6-0.3-2FT

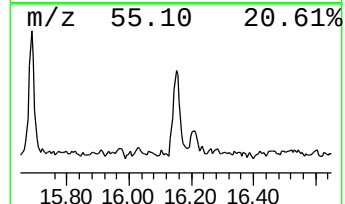
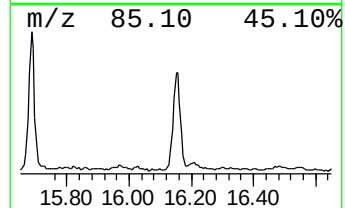
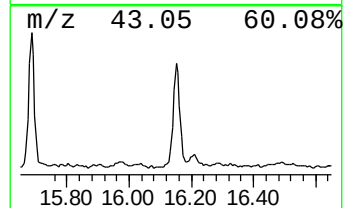
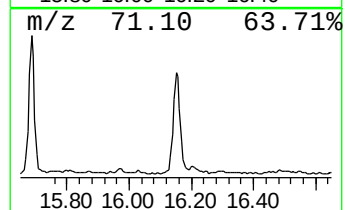
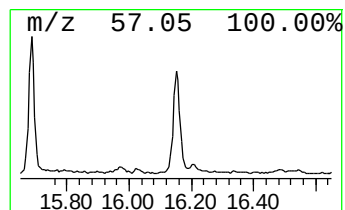
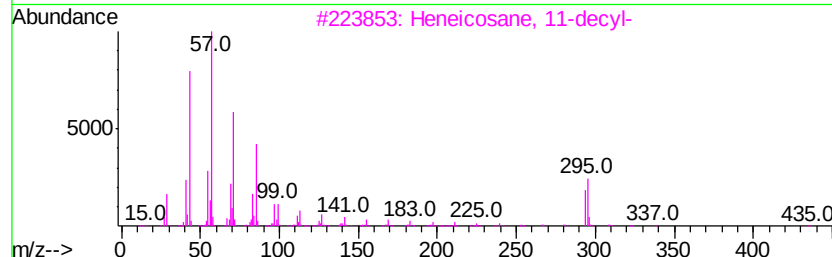
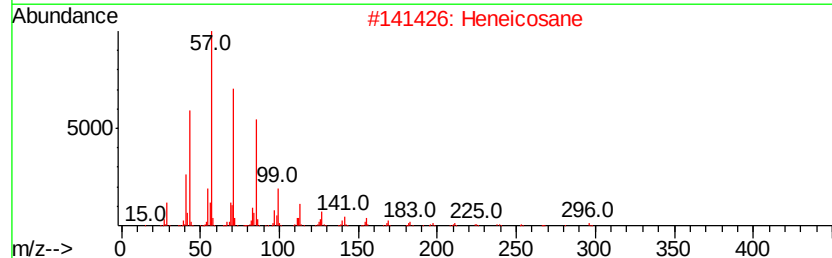
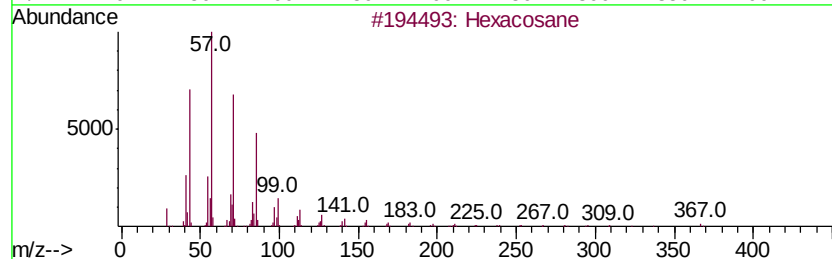
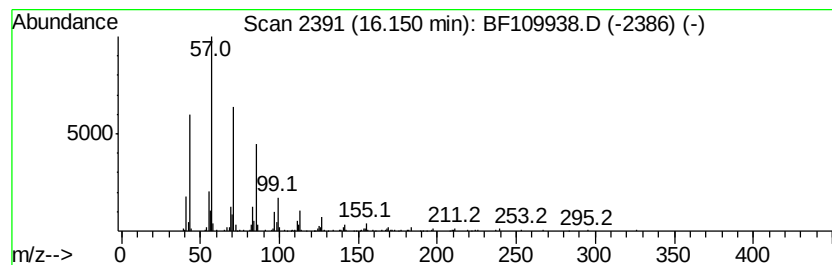
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	4.67 ng	488860	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	91
4		Triacontane	422	C30H62	000638-68-6	91
5		Heptacosane	380	C27H56	000593-49-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109938.D
Acq On : 17 Oct 2018 23:29
Operator : JU/SJ
Sample : J5539-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-6-0.3-2FT

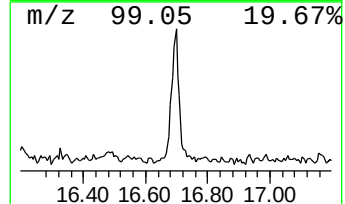
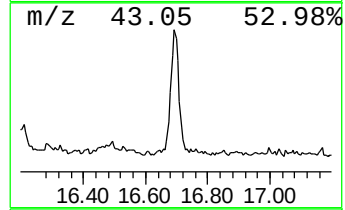
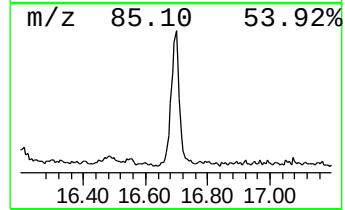
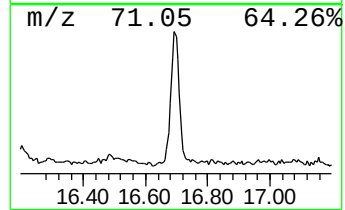
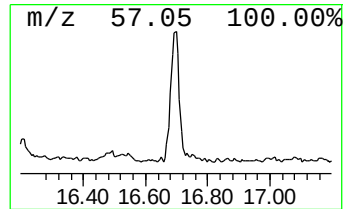
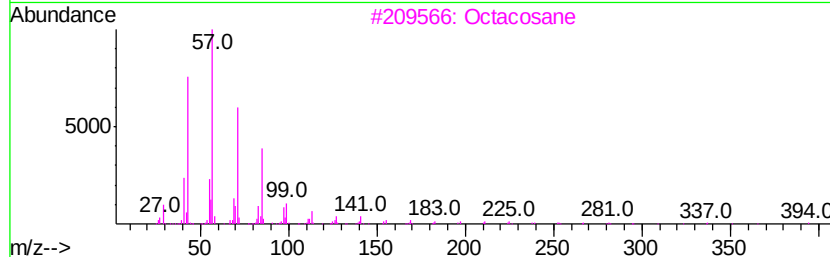
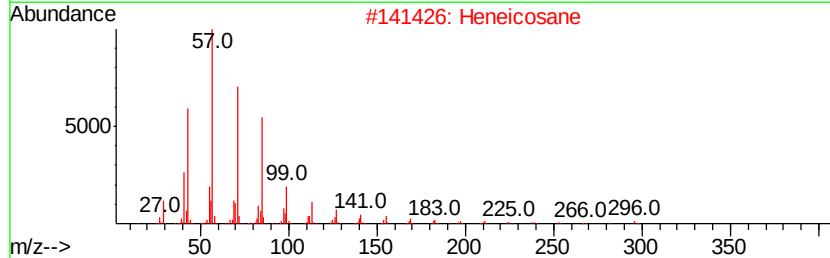
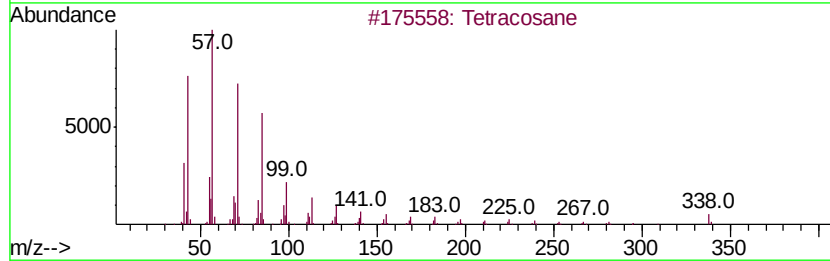
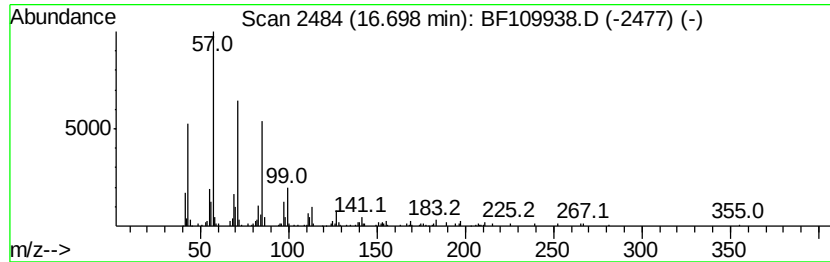
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.70	3.43 ng	358996	Perylene-d12	15.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Heneicosane	296	C21H44	000629-94-7	90
3			Octacosane	394	C28H58	000630-02-4	87
4			Hexacosane	366	C26H54	000630-01-3	87
5			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101718\
Data File : BF109938.D
Acq On : 17 Oct 2018 23:29
Operator : JU/SJ
Sample : J5539-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-6-0.3-2FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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...	2.32	10.9	ng	782528	1	6.97	1438150	20.0
2-Pentanone, 4-hy...	5.22	3.0	ng	211812	1	6.97	1438150	20.0
unknown6.75	6.75	64.3	ng	4624570	1	6.97	1438150	20.0
Heptadecyl heptaf...	13.97	5.1	ng	392800	5	14.15	1546480	20.0
Heneicosane	14.60	3.3	ng	252163	5	14.15	1546480	20.0
Triacontane	14.93	3.8	ng	401400	6	15.68	2094150	20.0
Hexacosane	16.15	4.7	ng	488860	6	15.68	2094150	20.0
Tetracosane	16.70	3.4	ng	358996	6	15.68	2094150	20.0