

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102518\
 Data File : BF110156.D
 Acq On : 25 Oct 2018 12:45
 Operator : JU/SJ
 Sample : J5618-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SSSI-1018-S-DH-14

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-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	2.122	4	6	21	rVB	284794	452114	12.19%	1.281%
2	2.334	37	42	50	rVB	354272	479890	12.94%	1.359%
3	5.210	527	531	538	rBV	134344	157322	4.24%	0.446%
4	5.592	591	596	599	rBV	3171285	2910142	78.44%	8.244%
5	6.592	759	766	770	rBV2	2812625	3366254	90.74%	9.536%
6	6.733	786	790	794	rBV	3167737	3173326	85.54%	8.989%
7	6.963	826	829	833	rBV	1089314	1000812	26.98%	2.835%
8	7.122	852	856	859	rBV	2818786	2434201	65.61%	6.895%
9	7.528	920	925	928	rBV	2098592	2013287	54.27%	5.703%
10	8.251	1043	1048	1051	rBV	1476282	1307853	35.25%	3.705%
11	9.327	1225	1231	1234	rBV	3830586	3709830	100.00%	10.509%
12	9.716	1293	1297	1302	rBV	400513	344789	9.29%	0.977%
13	10.010	1343	1347	1351	rBV	1706531	1467344	39.55%	4.157%
14	10.804	1477	1482	1485	rBV	2094265	2100281	56.61%	5.949%
15	11.504	1597	1601	1604	rBV	1520647	1382549	37.27%	3.916%
16	12.010	1682	1687	1692	rBV	240809	227557	6.13%	0.645%
17	12.715	1803	1807	1812	rBV	32497	38243	1.03%	0.108%
18	12.798	1817	1821	1826	rBV	37529	47537	1.28%	0.135%
19	13.086	1866	1870	1873	rBV	3146563	2860530	77.11%	8.103%
20	13.557	1945	1950	1954	rBV	86049	128188	3.46%	0.363%
21	13.639	1960	1964	1967	rVB2	51850	58702	1.58%	0.166%
22	13.968	2016	2020	2033	rBV	233955	260183	7.01%	0.737%
23	14.145	2046	2050	2054	rBV	867297	827542	22.31%	2.344%
24	14.286	2070	2074	2081	rVB	167912	159332	4.29%	0.451%
25	14.592	2121	2126	2135	rBV	360086	373859	10.08%	1.059%
26	14.915	2175	2181	2188	rBV	533107	627999	16.93%	1.779%
27	15.268	2235	2241	2249	rBV	599135	741357	19.98%	2.100%
28	15.674	2303	2310	2319	rBV	1099501	1512721	40.78%	4.285%
29	16.133	2381	2388	2395	rBV	362536	560070	15.10%	1.587%
30	16.198	2395	2399	2406	rVB8	18206	38569	1.04%	0.109%
31	16.668	2472	2479	2488	rBV	155009	291936	7.87%	0.827%
32	17.297	2581	2586	2595	rVB3	51190	107796	2.91%	0.305%
33	17.850	2673	2680	2690	rVB3	49355	140091	3.78%	0.397%

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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

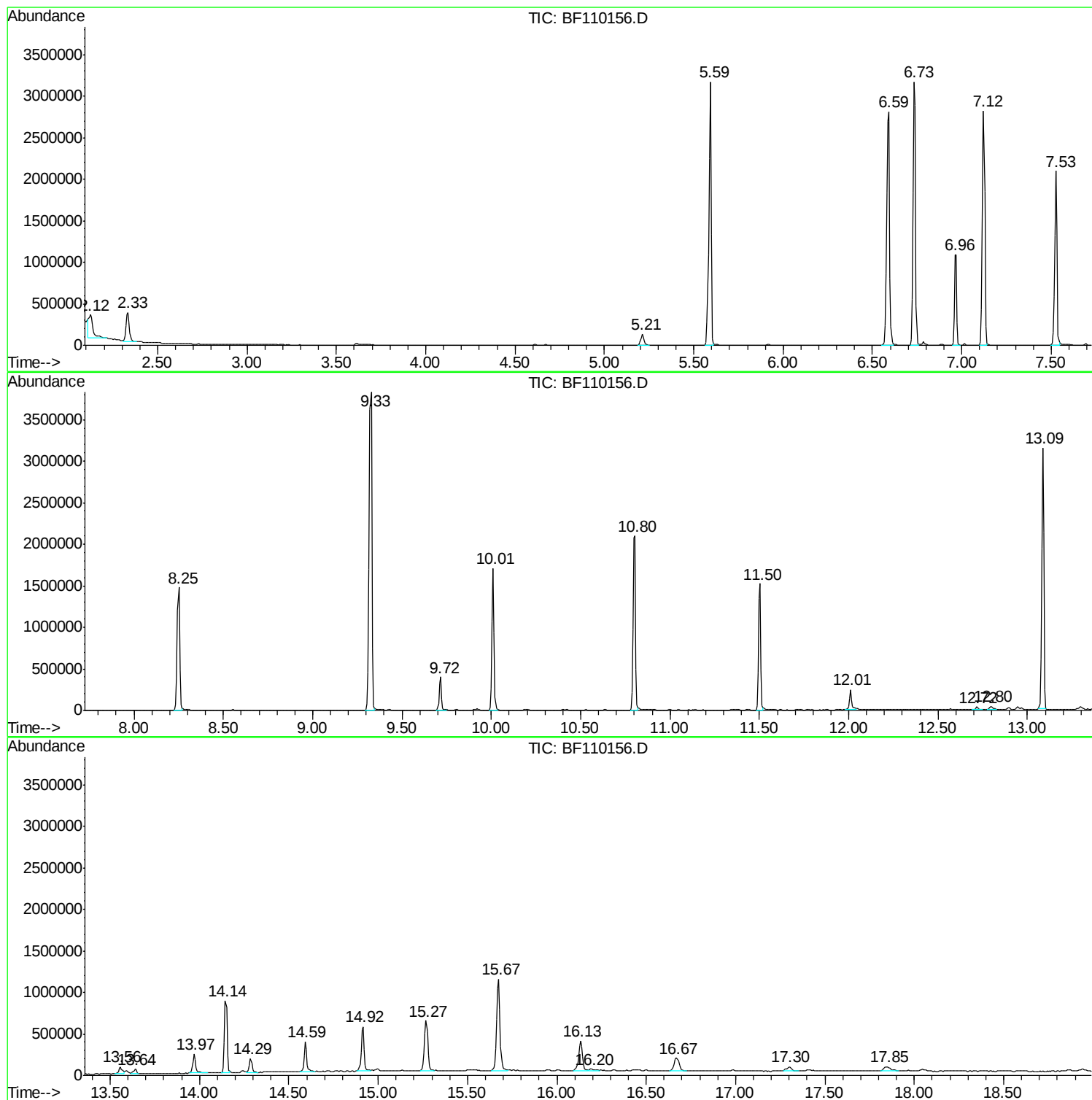
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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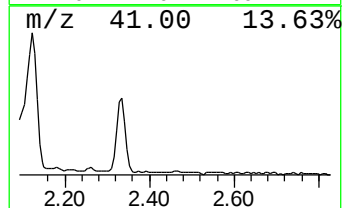
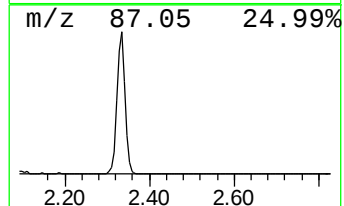
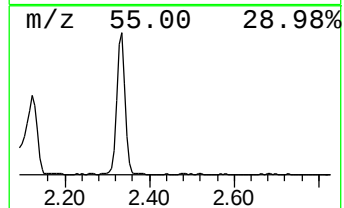
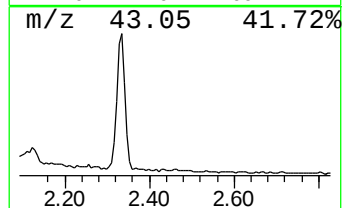
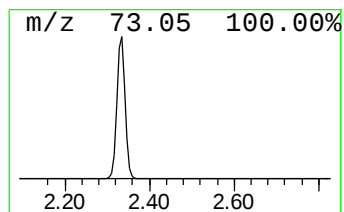
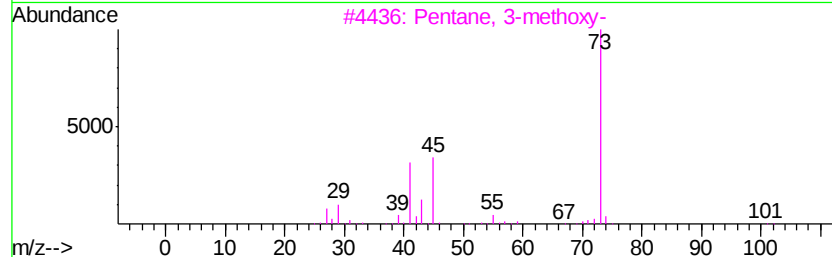
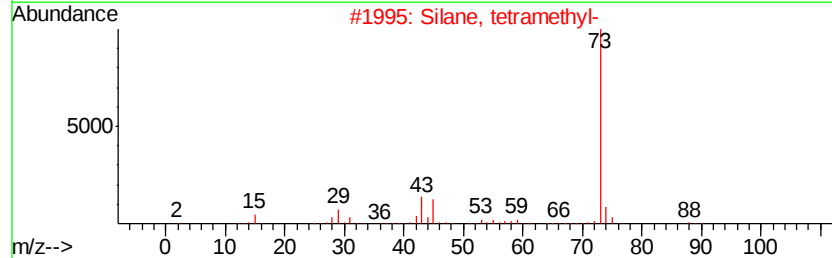
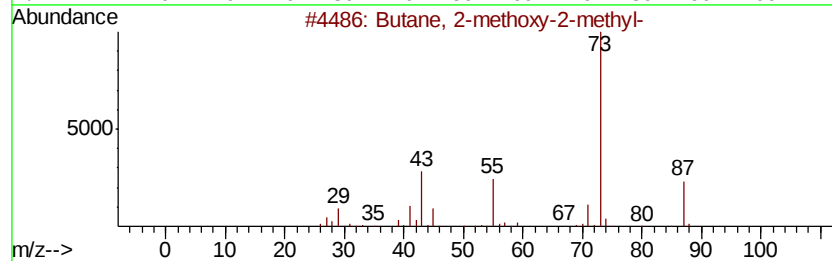
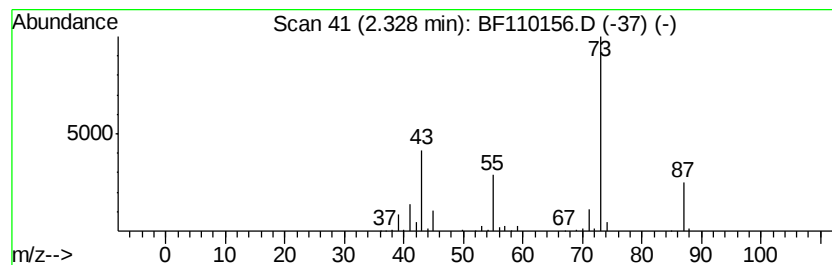
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	9.59 ng	479890	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		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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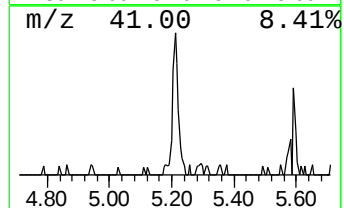
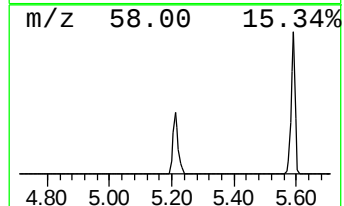
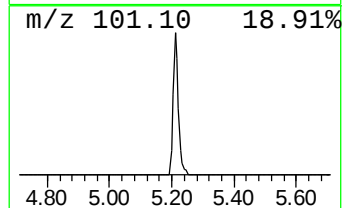
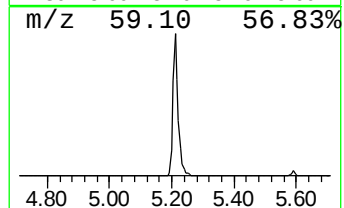
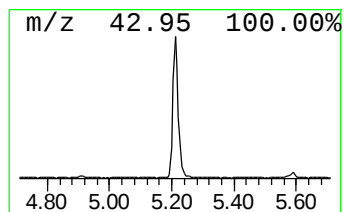
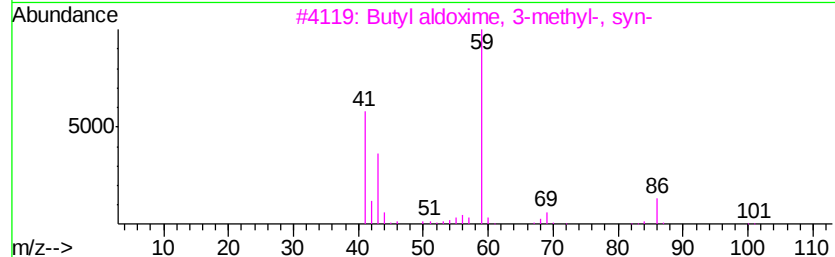
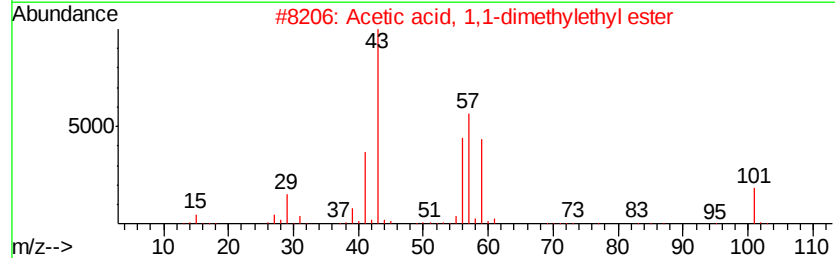
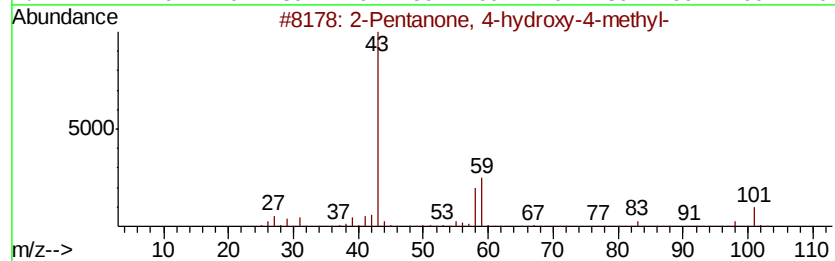
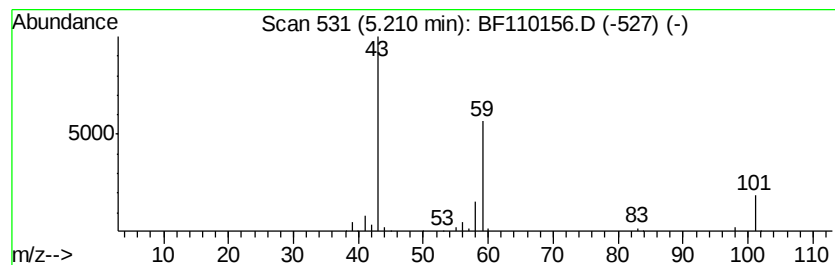
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	3.14 ng	157322	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9



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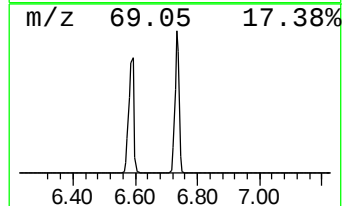
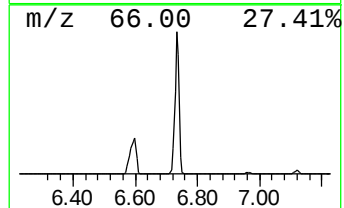
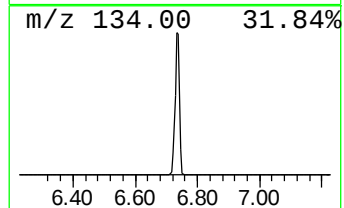
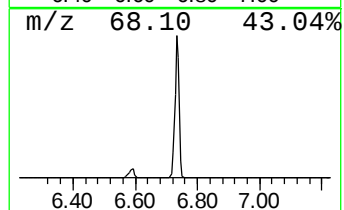
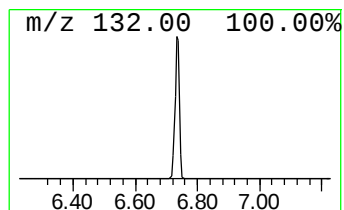
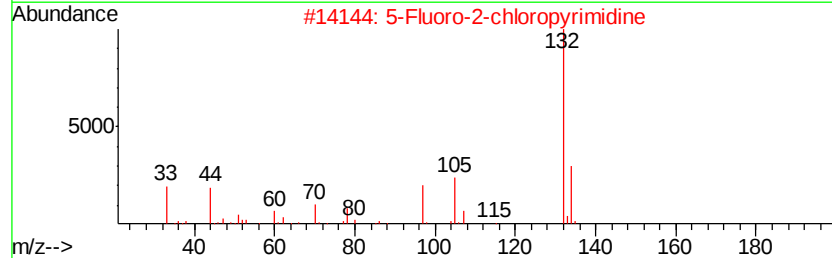
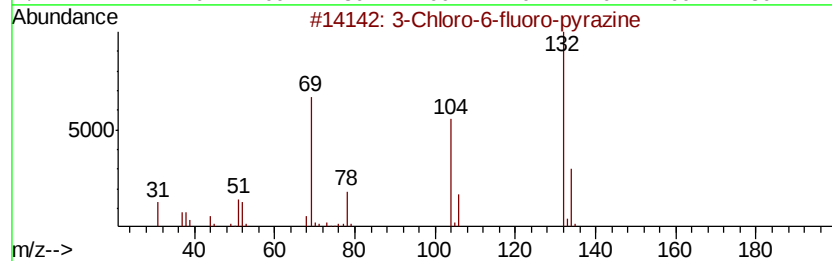
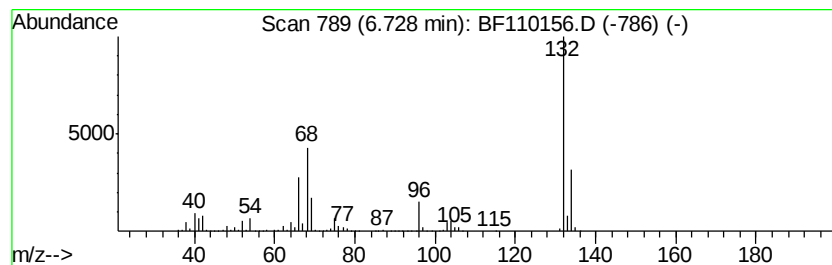
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	63.42 ng	3173330	1,4-Dichlorobenzene-d4	6.97

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	16
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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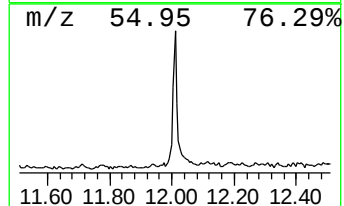
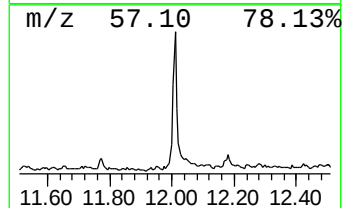
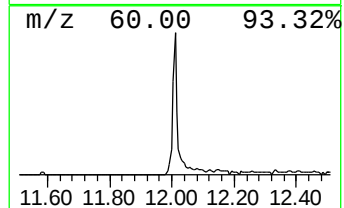
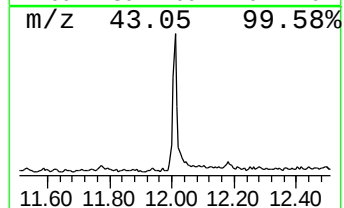
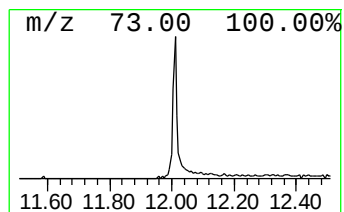
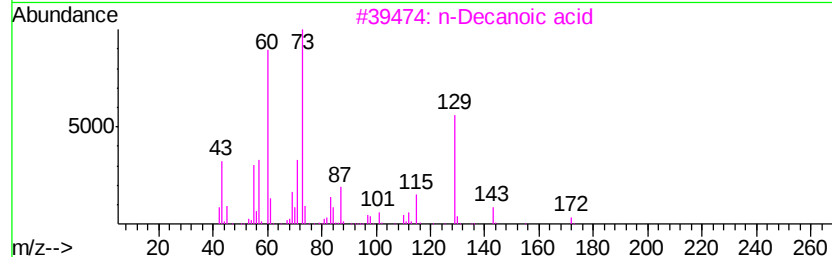
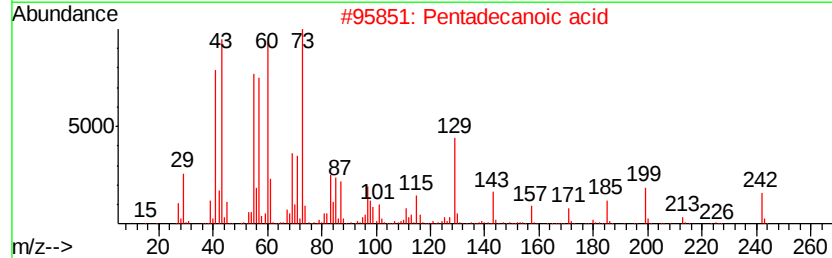
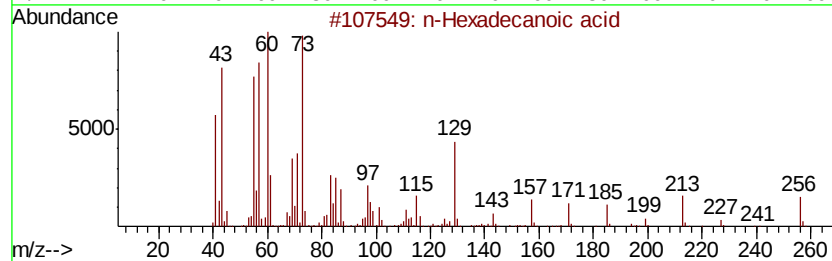
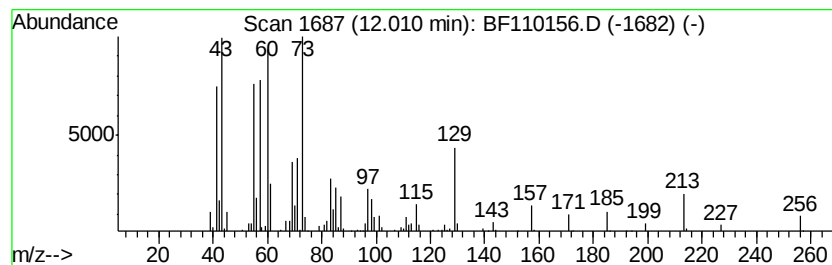
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	3.29 ng	227557	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		n-Decanoic acid	172	C10H20O2	000334-48-5	86
4		Tridecanoic acid	214	C13H26O2	000638-53-9	80
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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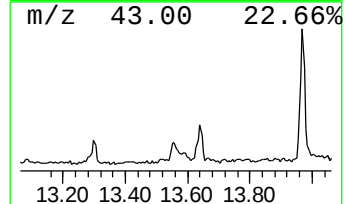
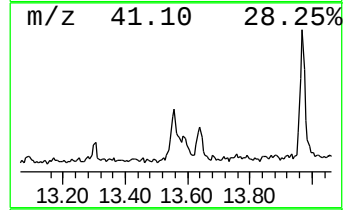
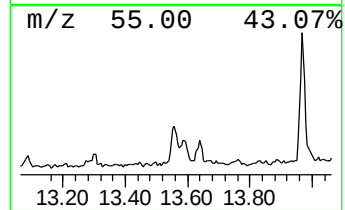
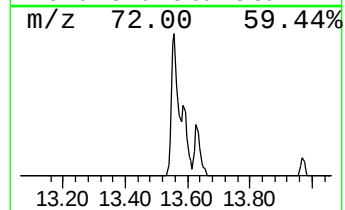
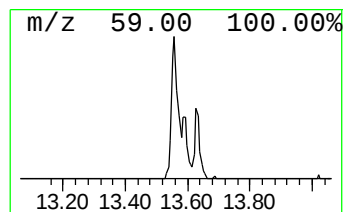
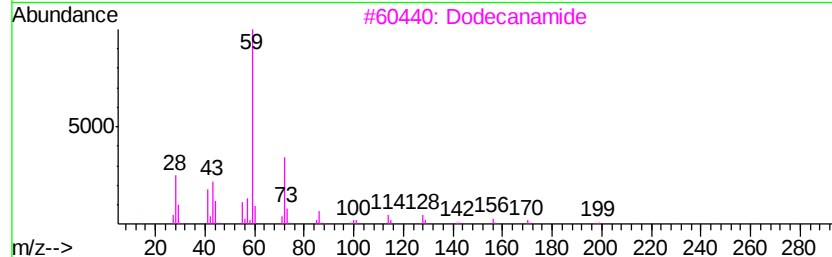
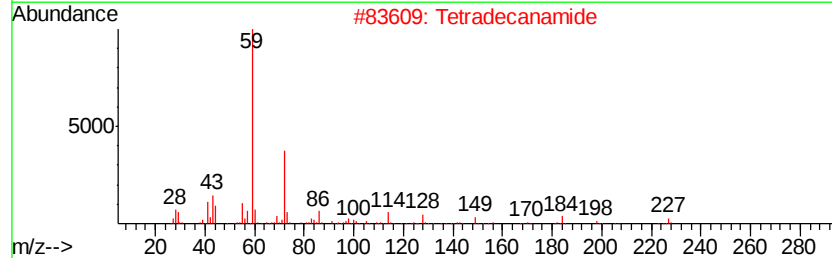
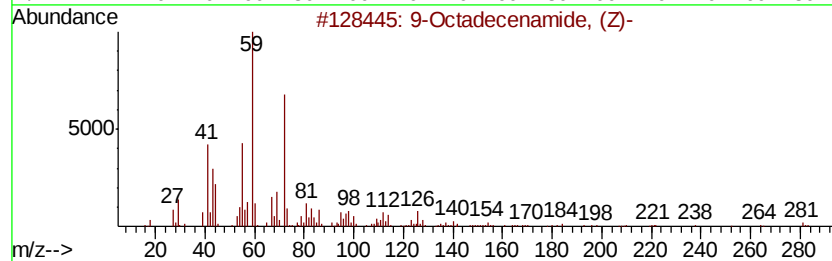
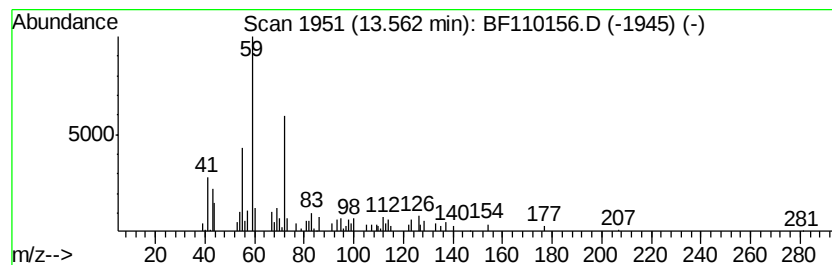
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TIC Integration Parameters: LSCINT.P

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.56	3.10 ng	128188	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		Tetradecanamide	227	C14H29NO	000638-58-4	53
3		Dodecanamide	199	C12H25NO	001120-16-7	53
4		Octanamide	143	C8H17NO	000629-01-6	50
5		Methyl 17-methoxy-10-methoxycarb...	386	C22H42O5	1000110-20-7	43



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Instrument :
BNA_F
ClientSampleId :
SSSI-1018-S-DH-14

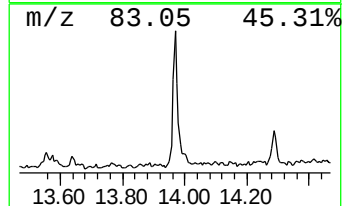
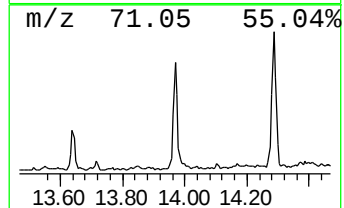
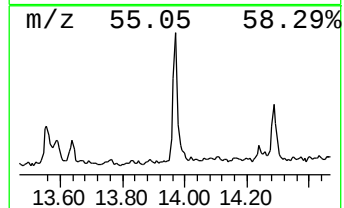
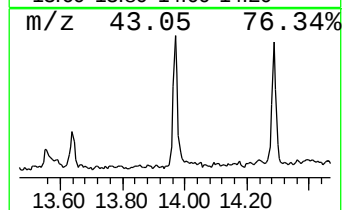
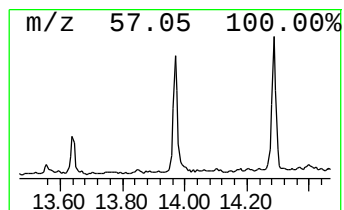
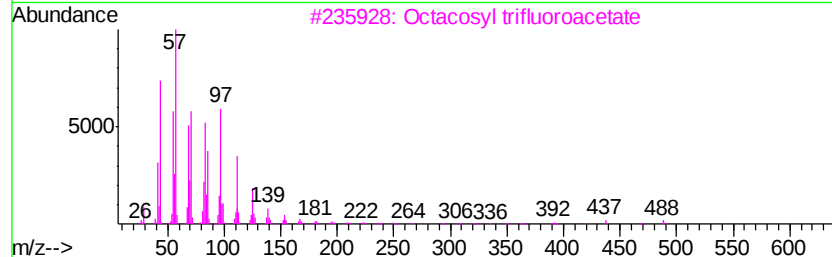
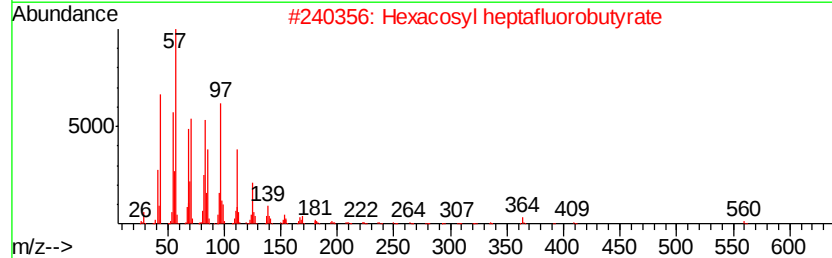
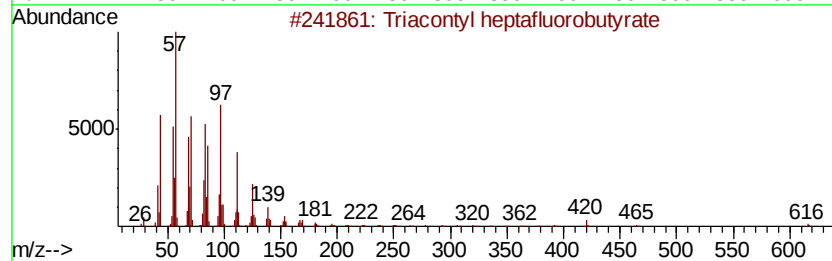
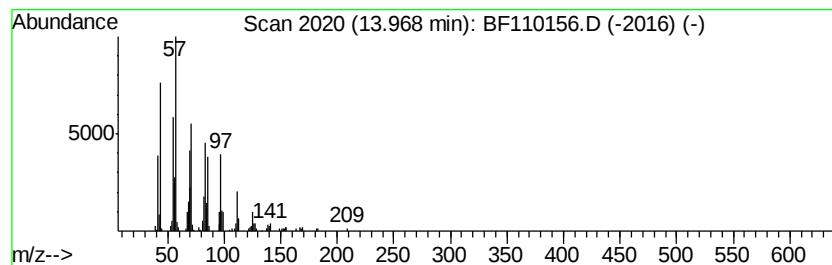
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triacontyl heptafluorobutyrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	6.29 ng	260183	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontyl heptafluorobutyrate	634	C34H61F7O2	1000351-83-2	91
2		Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	91
3		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
4		Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	91
5		Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102518\
Data File : BF110156.D
Acq On : 25 Oct 2018 12:45
Operator : JU/SJ
Sample : J5618-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

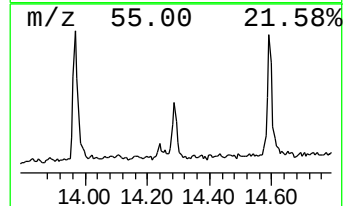
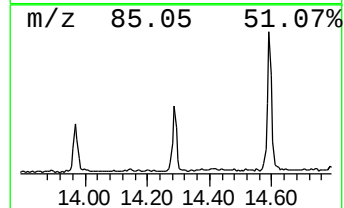
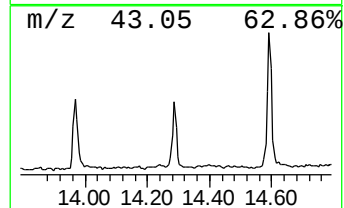
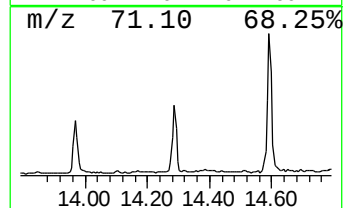
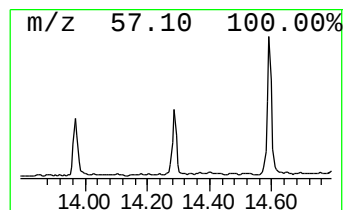
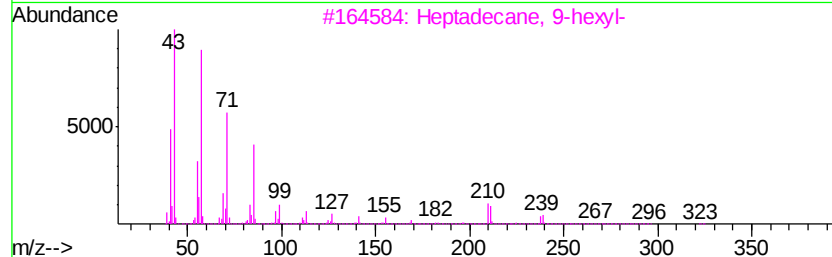
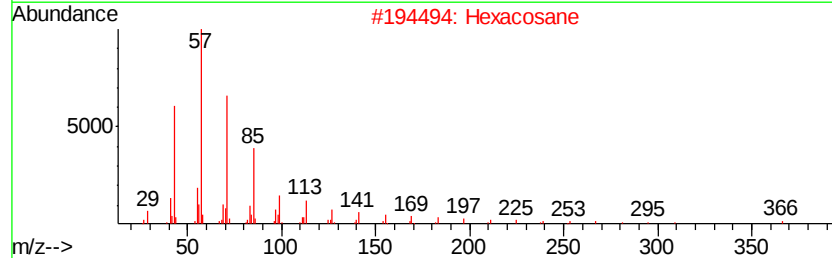
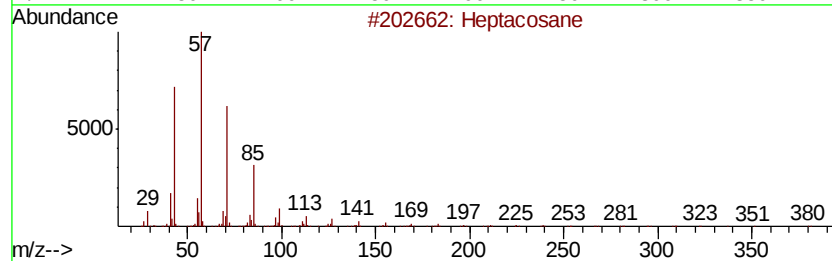
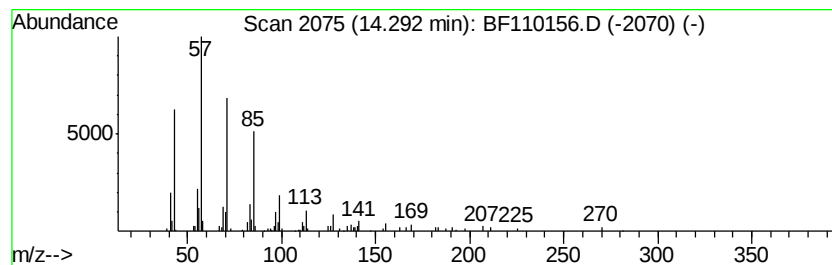
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ClientSampleId :
SSSI-1018-S-DH-14

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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 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	3.85 ng	159332	Chrysene-d12	14.14
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	91
2	Hexacosane	366 C26H54	000630-01-3	90
3	Heptadecane, 9-hexyl-	324 C23H48	055124-79-3	90
4	Hexadecane	226 C16H34	000544-76-3	86
5	Hexatriacontane	507 C36H74	000630-06-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102518\
Data File : BF110156.D
Acq On : 25 Oct 2018 12:45
Operator : JU/SJ
Sample : J5618-04
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
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SSSI-1018-S-DH-14

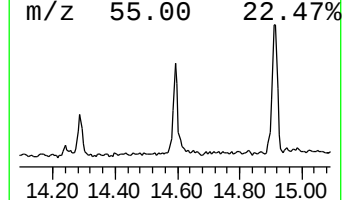
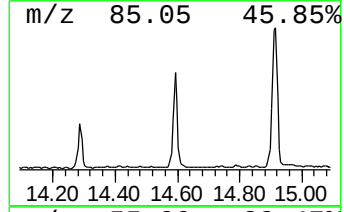
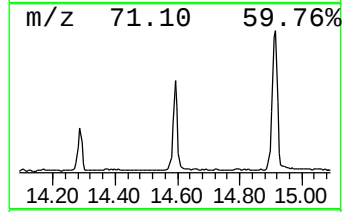
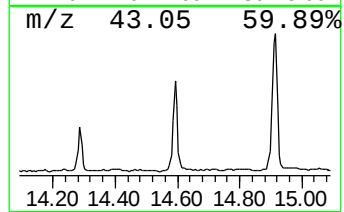
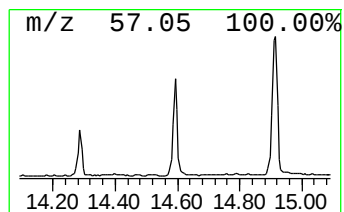
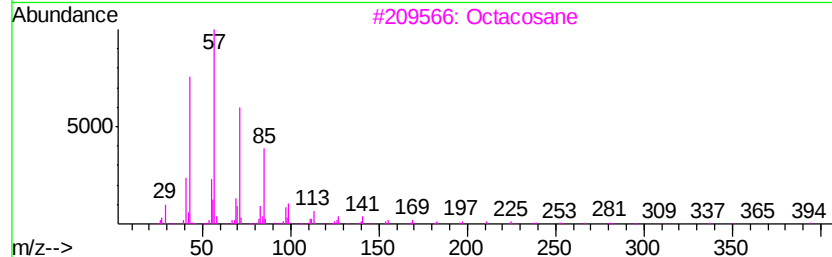
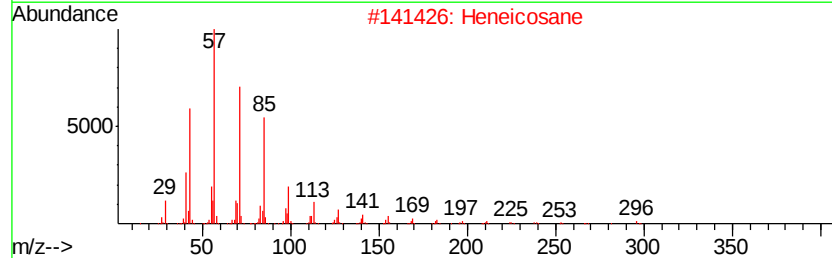
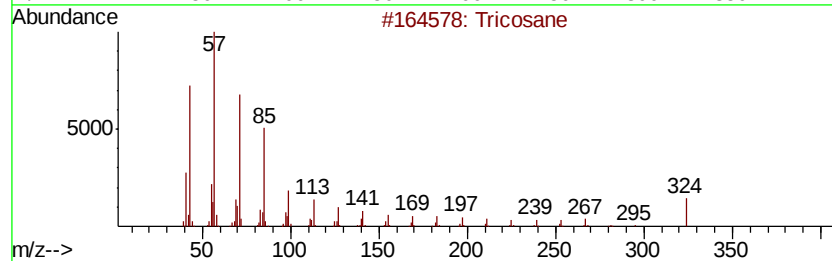
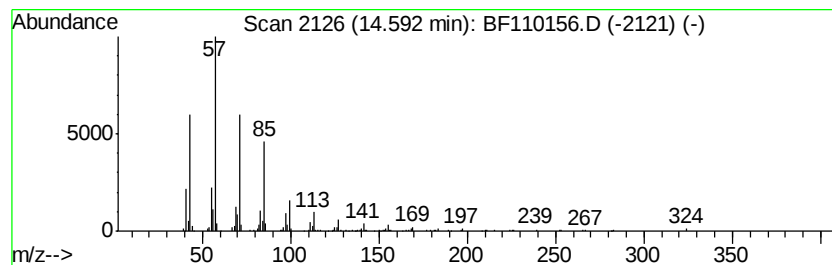
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tricosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	9.04 ng	373859	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricosane	324	C23H48	000638-67-5	93
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Docosane	310	C22H46	000629-97-0	90
5		Triacontane	422	C30H62	000638-68-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102518\
Data File : BF110156.D
Acq On : 25 Oct 2018 12:45
Operator : JU/SJ
Sample : J5618-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SSSI-1018-S-DH-14

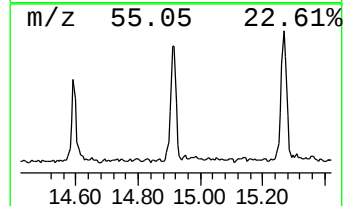
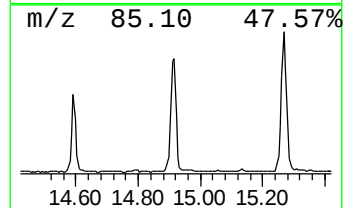
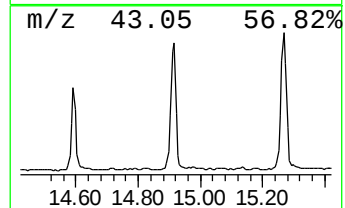
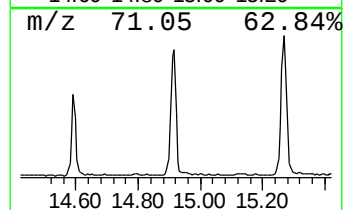
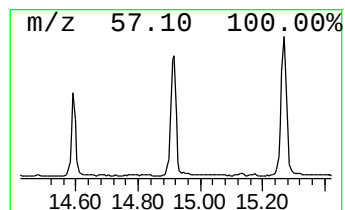
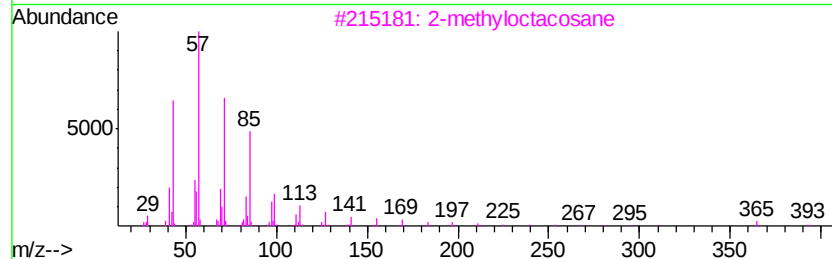
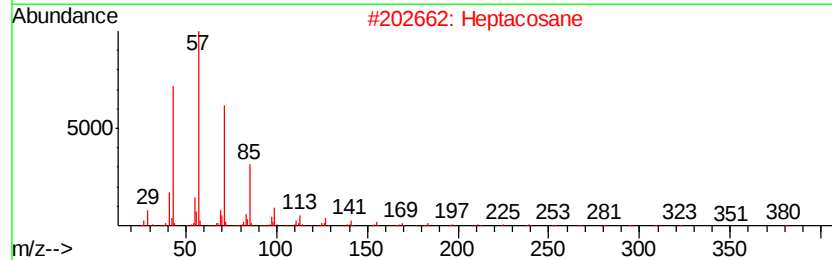
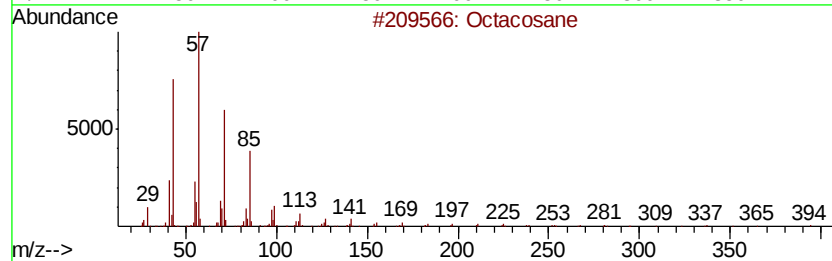
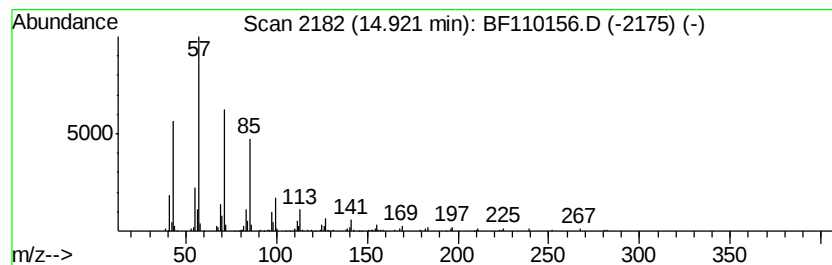
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	8.30 ng	627999	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Docosane	310	C22H46	000629-97-0	91
5		Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102518\
Data File : BF110156.D
Acq On : 25 Oct 2018 12:45
Operator : JU/SJ
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Misc :
ALS Vial : 5 Sample Multiplier: 1

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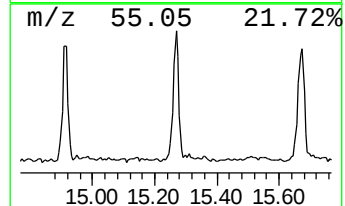
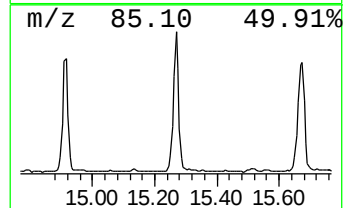
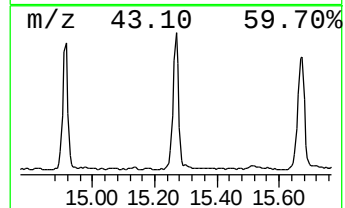
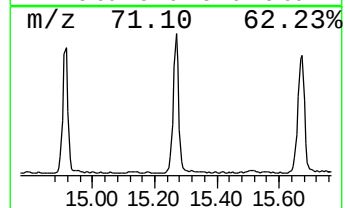
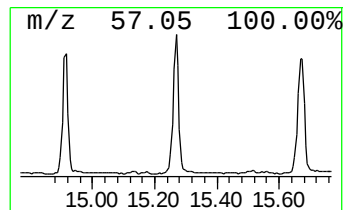
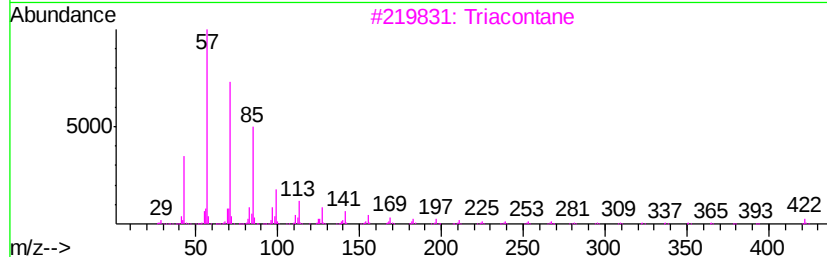
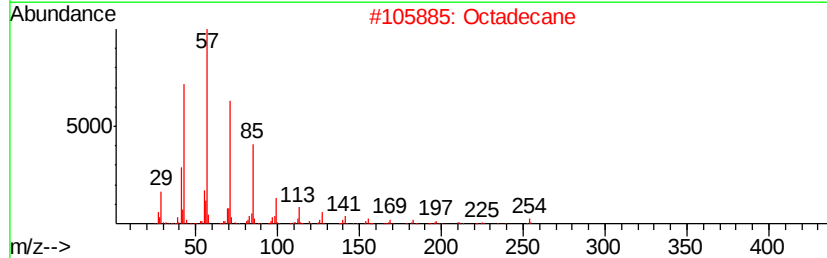
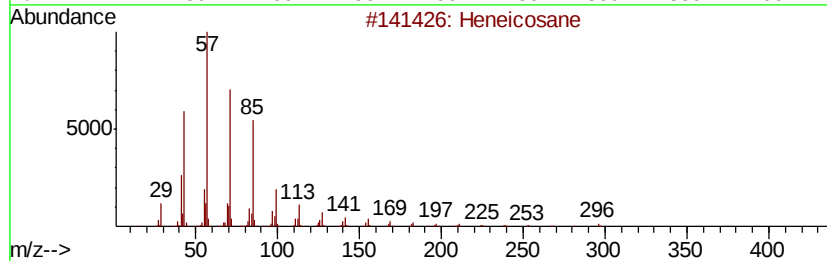
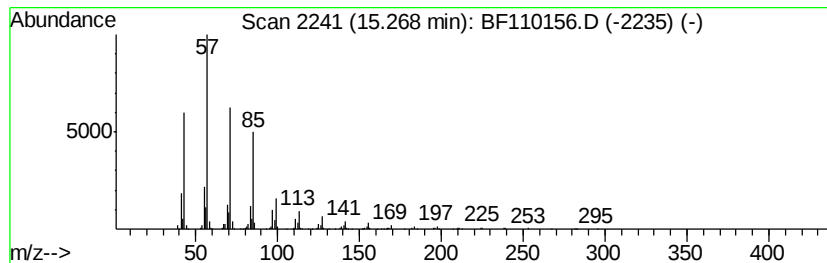
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	9.80 ng	741357	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Octadecane	254	C18H38	000593-45-3	90
3		Triacotane	422	C30H62	000638-68-6	90
4		Hexadecane	226	C16H34	000544-76-3	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102518\
Data File : BF110156.D
Acq On : 25 Oct 2018 12:45
Operator : JU/SJ
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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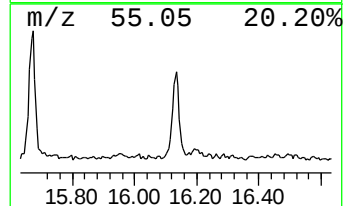
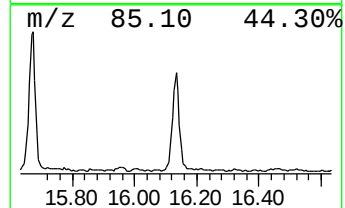
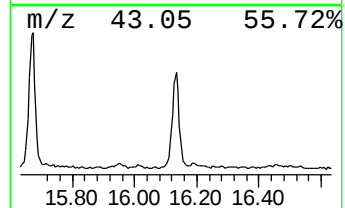
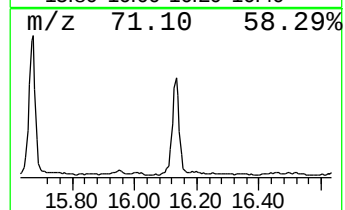
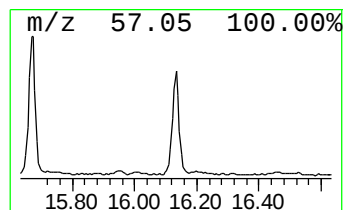
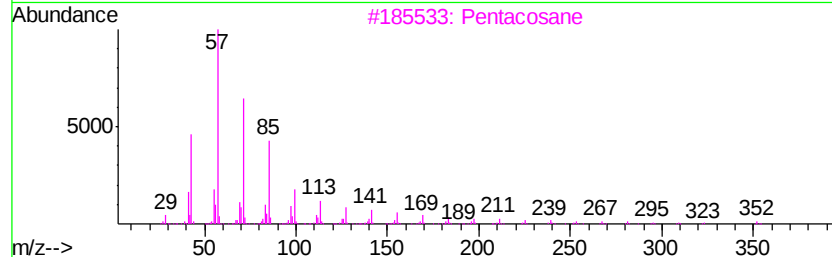
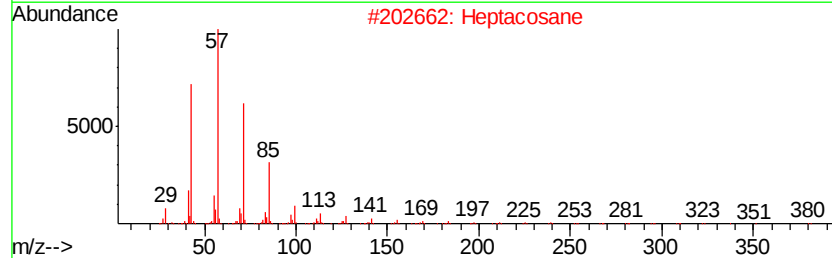
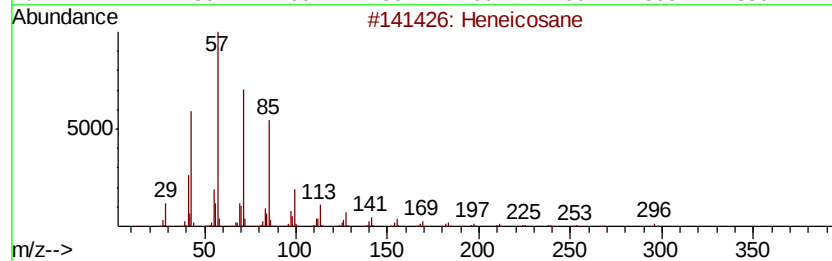
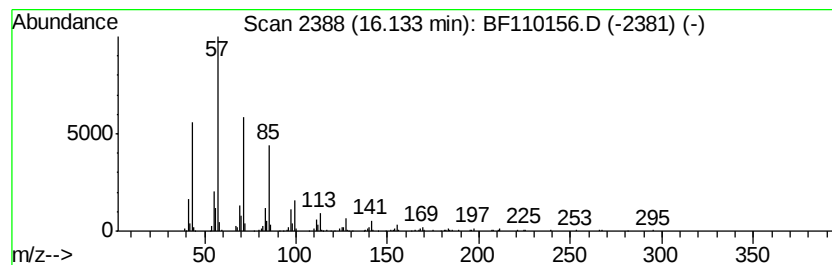
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	7.40 ng	560070	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Pentacosane	352	C25H52	000629-99-2	91
4		Tetracosane	338	C24H50	000646-31-1	90
5		2-methyloctacosane	408	C29H60	1000376-72-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102518\
Data File : BF110156.D
Acq On : 25 Oct 2018 12:45
Operator : JU/SJ
Sample : J5618-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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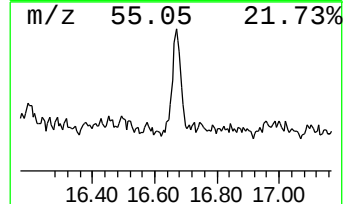
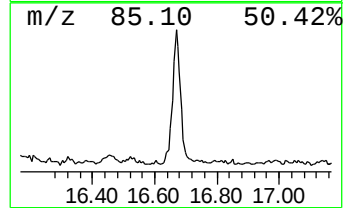
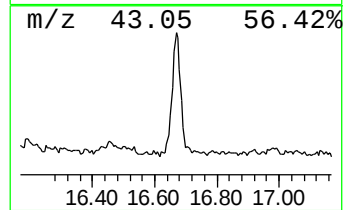
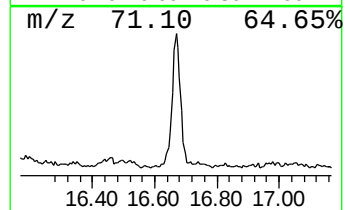
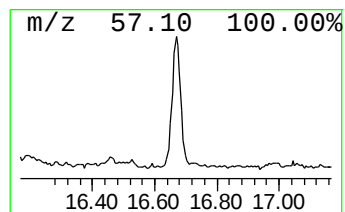
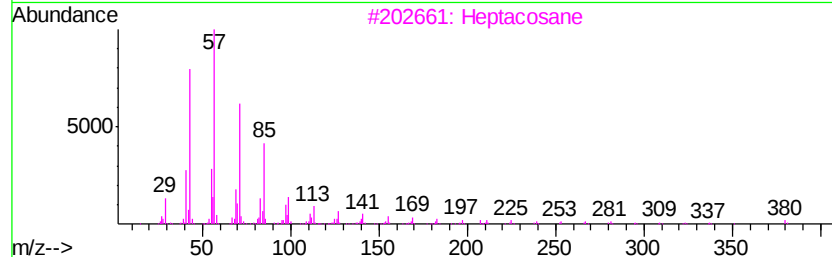
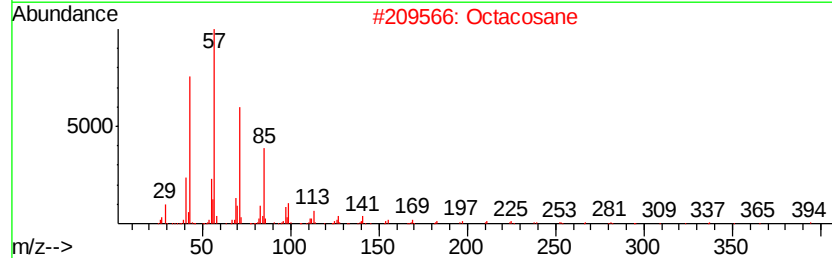
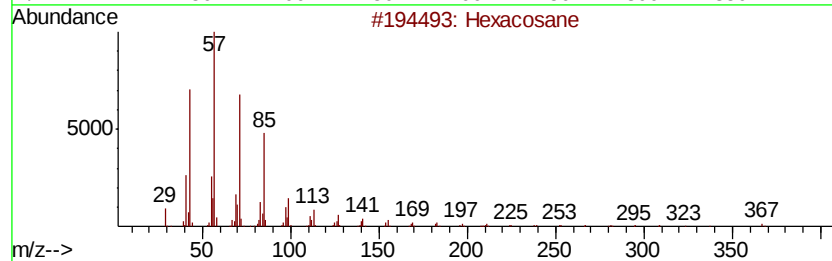
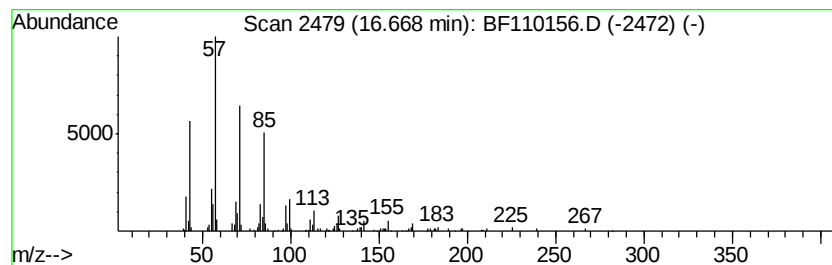
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.67	3.86 ng	291936	Perylene-d12	15.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	93
2			Octacosane	394	C28H58	000630-02-4	91
3			Heptacosane	380	C27H56	000593-49-7	91
4			2-methyloctacosane	408	C29H60	1000376-72-8	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102518\
Data File : BF110156.D
Acq On : 25 Oct 2018 12:45
Operator : JU/SJ
Sample : J5618-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SSSI-1018-S-DH-14

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
Butane, 2-methoxy...	2.33	9.6	ng	479890	1	6.97	1000810	20.0
2-Pentanone, 4-hy...	5.21	3.1	ng	157322	1	6.97	1000810	20.0
unknown6.73	6.73	63.4	ng	3173330	1	6.97	1000810	20.0
n-Hexadecanoic acid	12.01	3.3	ng	227557	4	11.50	1382550	20.0
9-Octadecenamide,...	13.56	3.1	ng	128188	5	14.14	827542	20.0
Triacontyl heptaf...	13.97	6.3	ng	260183	5	14.14	827542	20.0
Heptacosane	14.29	3.9	ng	159332	5	14.14	827542	20.0
Tricosane	14.59	9.0	ng	373859	5	14.14	827542	20.0
Octacosane	14.92	8.3	ng	627999	6	15.67	1512720	20.0
Heneicosane	15.27	9.8	ng	741357	6	15.67	1512720	20.0
Pentacosane	16.13	7.4	ng	560070	6	15.67	1512720	20.0
Hexacosane	16.67	3.9	ng	291936	6	15.67	1512720	20.0