

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
 Data File : BF111851.D
 Acq On : 4 Jan 2019 18:14
 Operator : JU/SJ
 Sample : K1018-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

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-BF121918.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

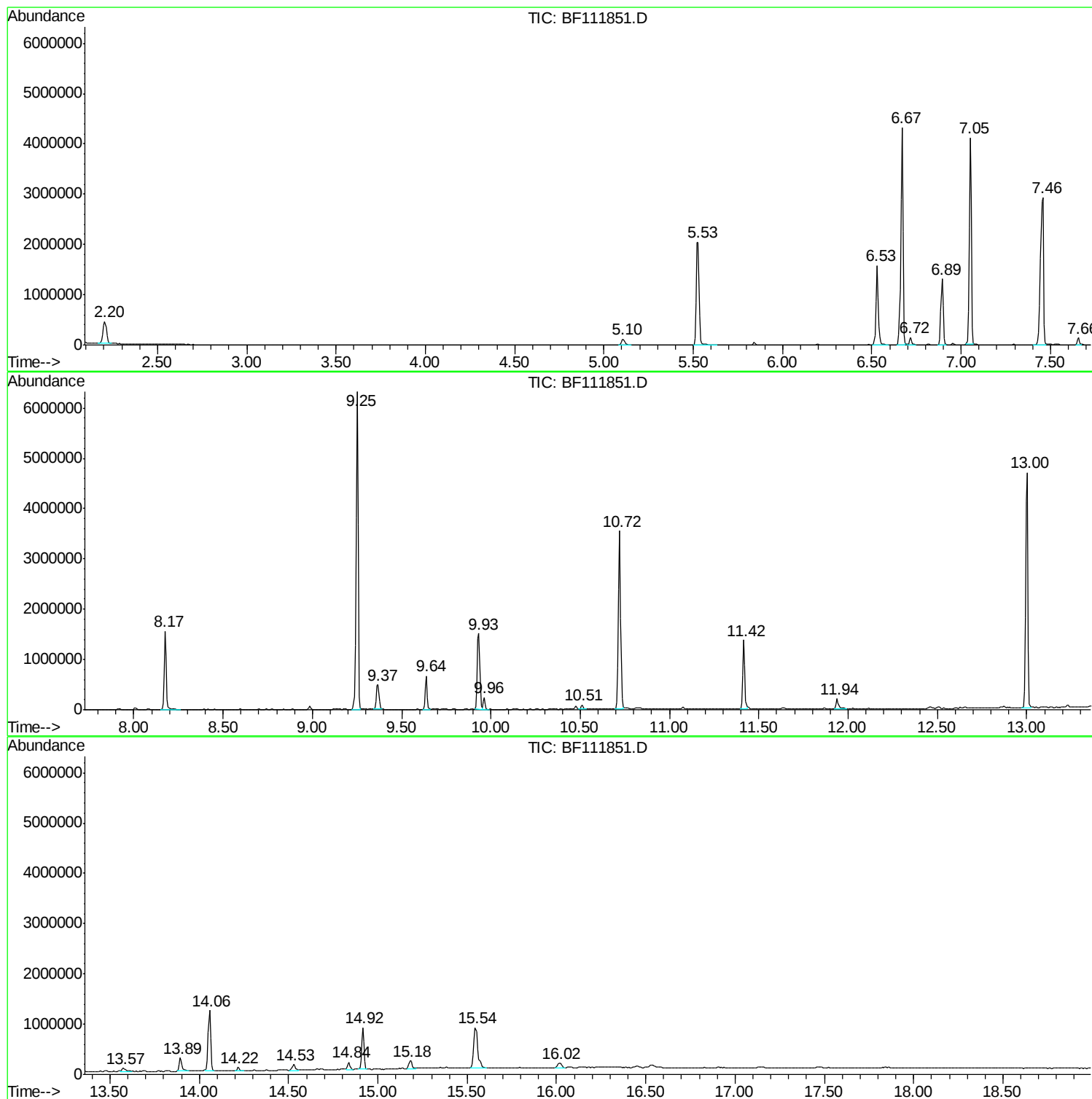
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	13	20	26	rVB	436639	556512	10.05%	1.436%
2	5.104	509	513	521	rVB	117451	133229	2.41%	0.344%
3	5.528	580	585	602	rBV	2046449	2057527	37.16%	5.311%
4	6.528	751	755	766	rBV2	1575029	1481690	26.76%	3.824%
5	6.669	774	779	782	rBV	4318976	3879422	70.07%	10.013%
6	6.716	784	787	792	rVB	144879	127650	2.31%	0.329%
7	6.893	813	817	821	rBV	1305363	1056941	19.09%	2.728%
8	7.051	840	844	847	rBV	4116097	3677958	66.43%	9.493%
9	7.457	904	913	916	rBV	2931222	3206937	57.92%	8.278%
10	7.657	944	947	950	rBV	135902	117755	2.13%	0.304%
11	8.175	1031	1035	1049	rBV	1556563	1344816	24.29%	3.471%
12	9.251	1213	1218	1221	rBV	6320773	5536414	100.00%	14.290%
13	9.369	1233	1238	1241	rBV	487779	475234	8.58%	1.227%
14	9.639	1280	1284	1287	rBV	668934	525757	9.50%	1.357%
15	9.933	1330	1334	1337	rBV	1503026	1395729	25.21%	3.603%
16	9.963	1337	1339	1343	rVB	243171	182203	3.29%	0.470%
17	10.510	1429	1432	1436	rBV	85001	74992	1.35%	0.194%
18	10.722	1463	1468	1471	rBV	3538910	3157111	57.02%	8.149%
19	11.416	1582	1586	1589	rBV	1371316	1139089	20.57%	2.940%
20	11.939	1672	1675	1684	rBV2	197115	194272	3.51%	0.501%
21	13.004	1851	1856	1859	rBV	4678759	4300680	77.68%	11.101%
22	13.574	1950	1953	1961	rVB3	70814	103407	1.87%	0.267%
23	13.892	2004	2007	2015	rBV2	261395	311091	5.62%	0.803%
24	14.057	2031	2035	2039	rVB	1196673	1037096	18.73%	2.677%
25	14.216	2059	2062	2067	rBV	72750	67059	1.21%	0.173%
26	14.527	2111	2115	2120	rBV	115302	129700	2.34%	0.335%
27	14.839	2165	2168	2171	rVB	151337	140407	2.54%	0.362%
28	14.916	2177	2181	2185	rVB	822581	816760	14.75%	2.108%
29	15.180	2223	2226	2232	rBV	153591	173908	3.14%	0.449%
30	15.545	2283	2288	2298	rBV	797632	1195712	21.60%	3.086%
31	16.015	2364	2368	2373	rVB2	94021	145438	2.63%	0.375%

Sum of corrected areas: 38742496

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ALS Vial : 11 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121918.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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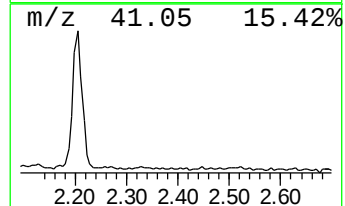
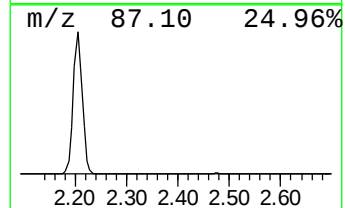
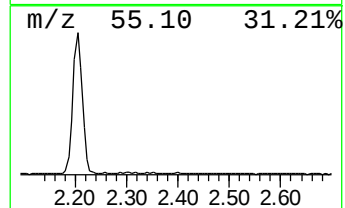
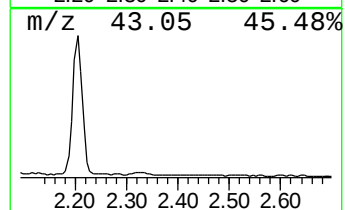
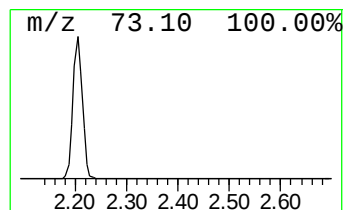
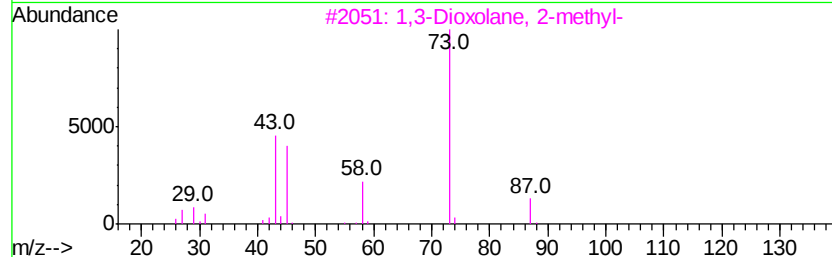
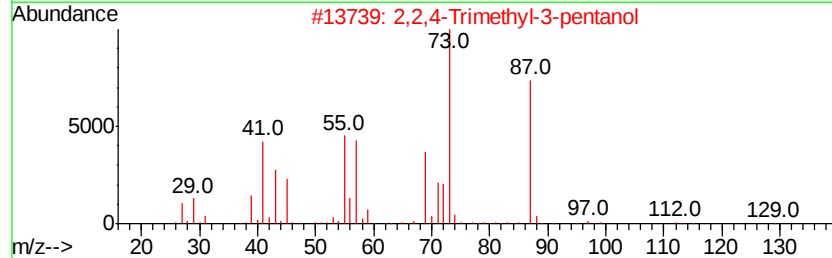
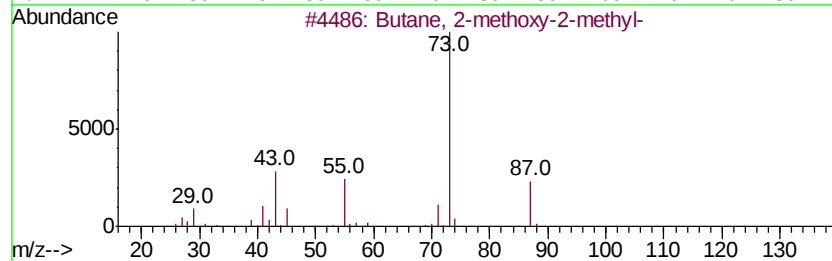
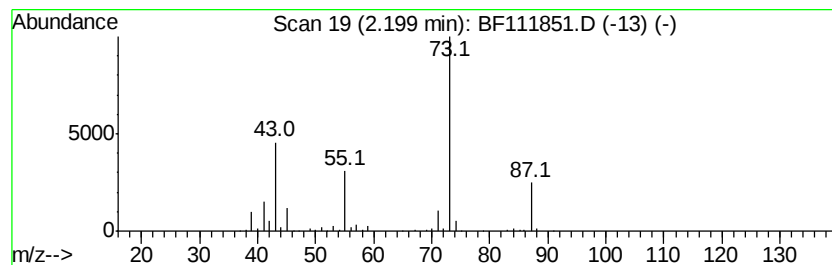
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	10.53 ng	556512	1,4-Dichlorobenzene-d4	6.89

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	32
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	23
5		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16



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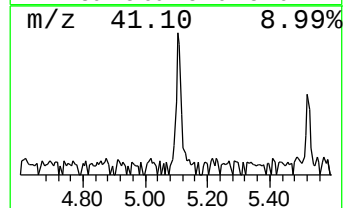
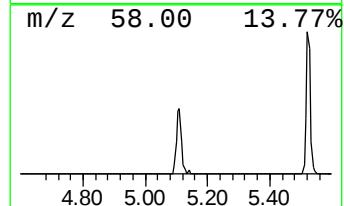
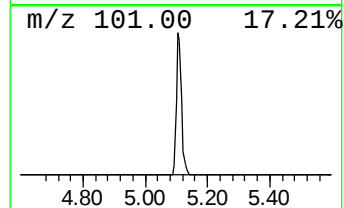
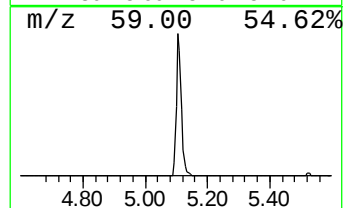
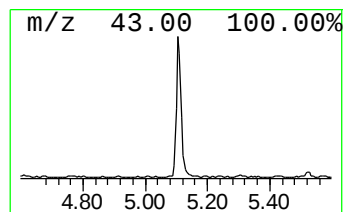
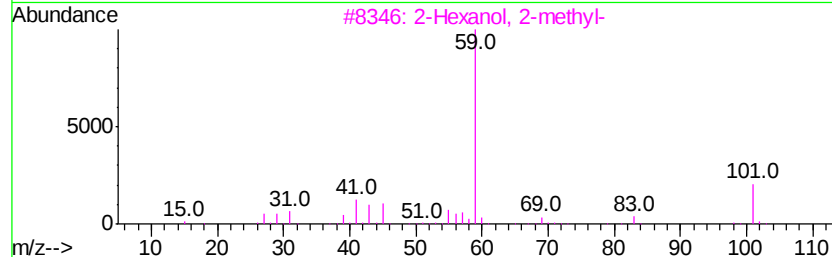
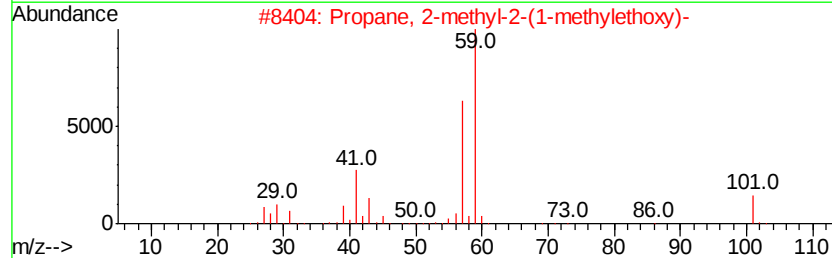
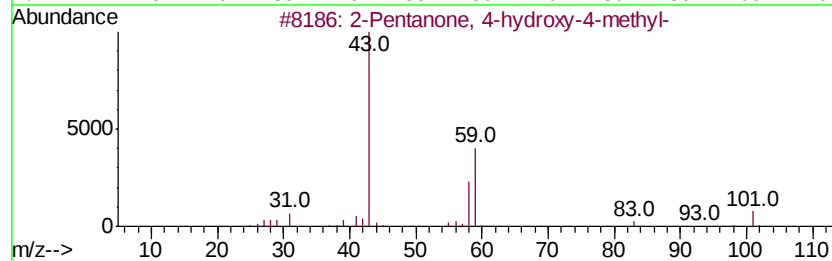
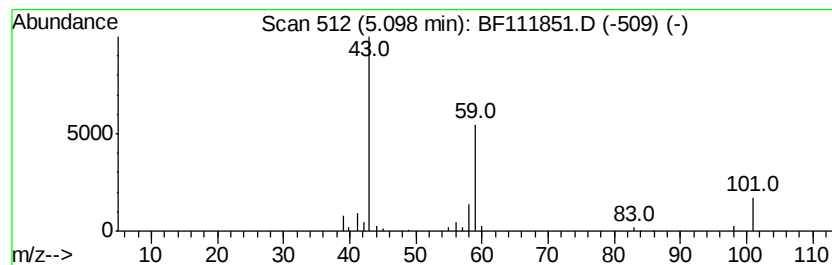
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	2.52 ng	133229	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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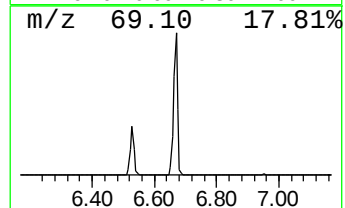
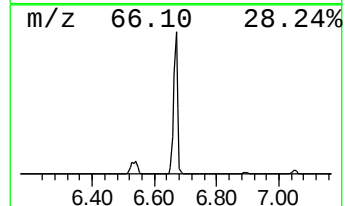
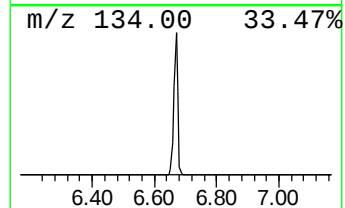
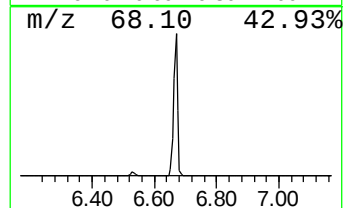
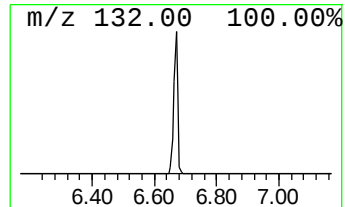
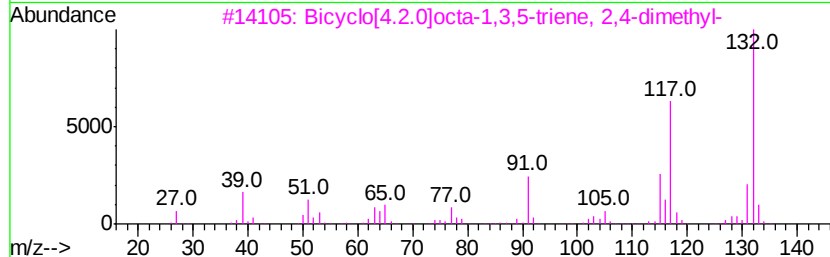
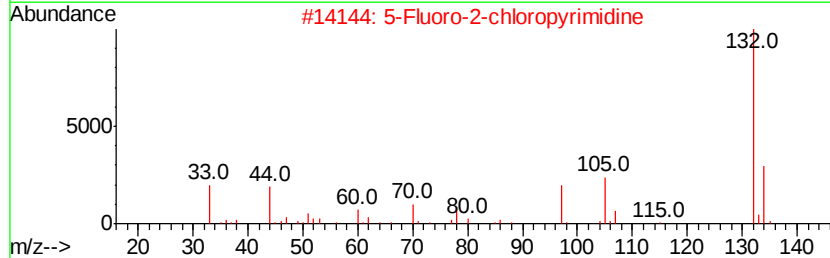
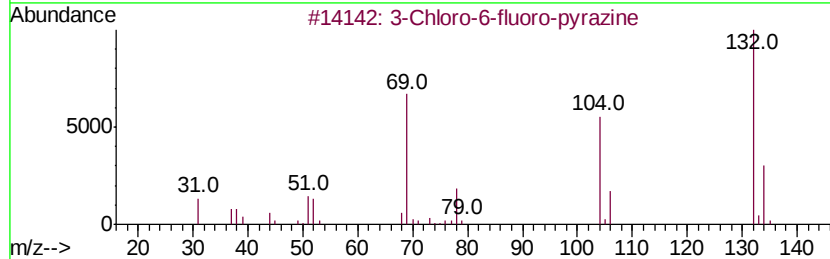
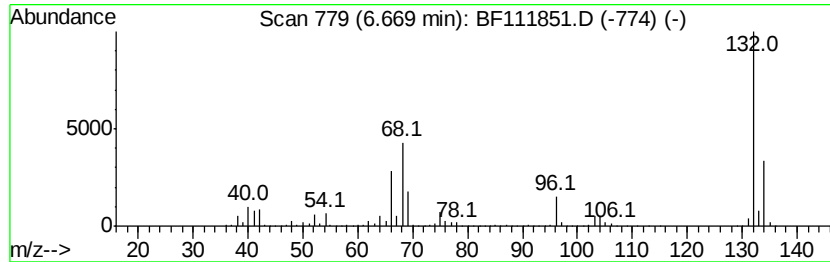
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Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	73.41 ng	3879420	1,4-Dichlorobenzene-d4	6.89

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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		Xenon	132	Xe	007440-63-3	9



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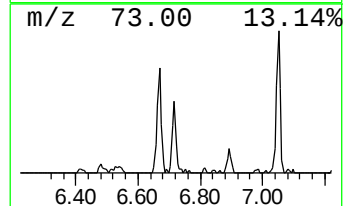
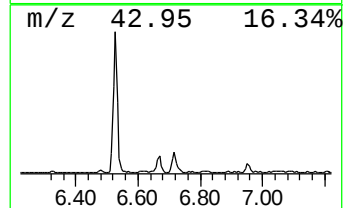
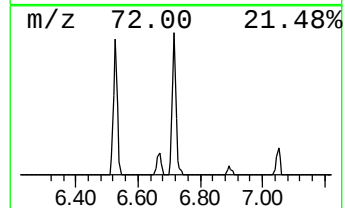
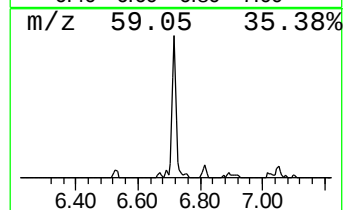
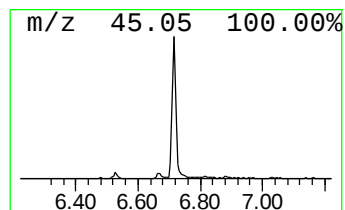
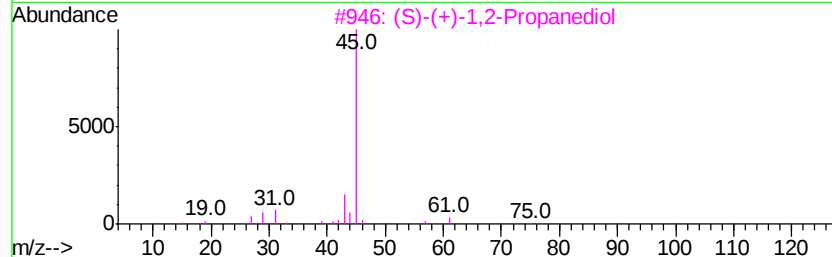
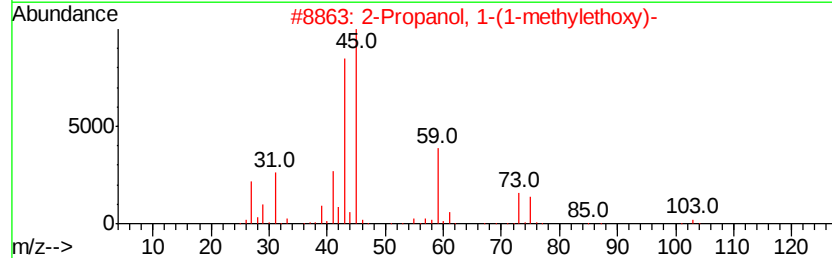
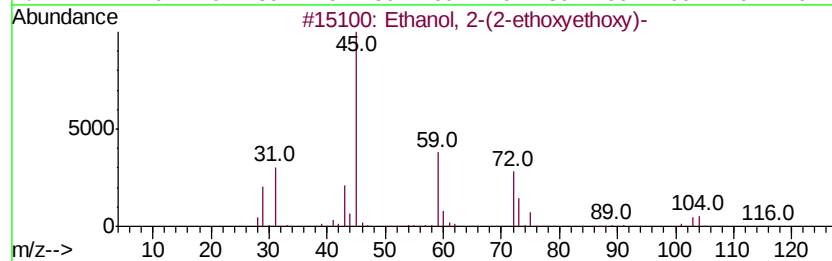
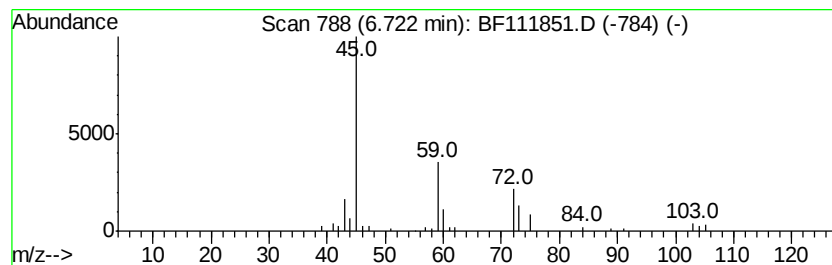
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	2.42 ng	127650	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
3			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	37
4			Ethanol, 2-[2-(2-propenyl)ethoxy]-	146	C7H14O3	015075-50-0	36
5			Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	9



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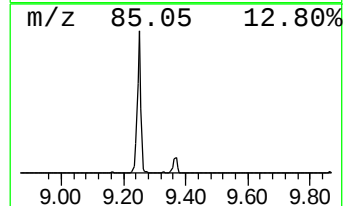
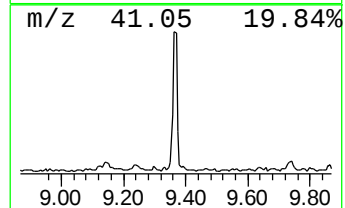
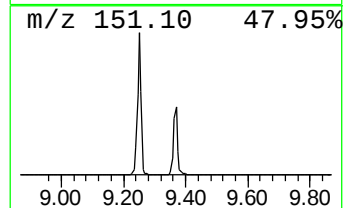
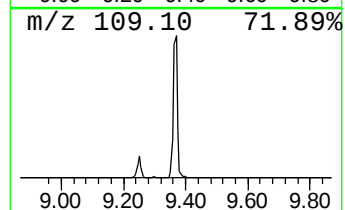
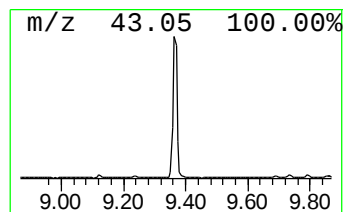
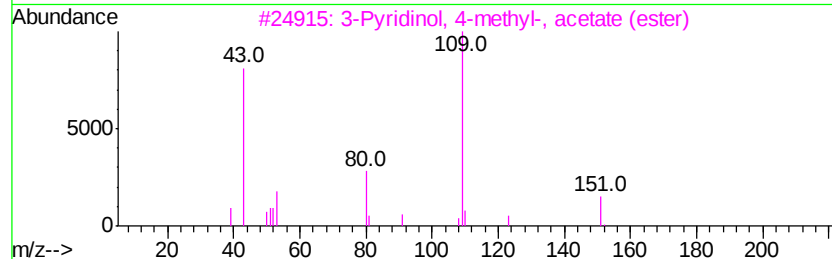
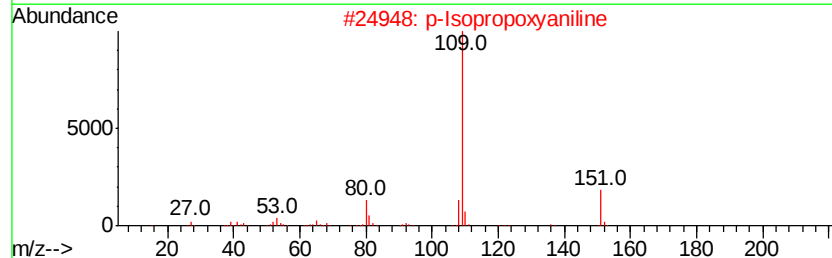
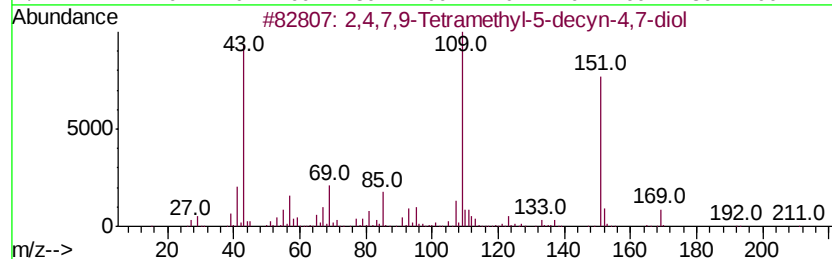
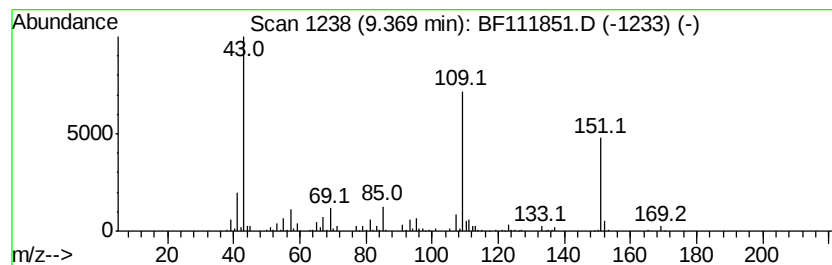
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.37	6.81 ng	475234	Acenaphthene-d10	9.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90		
2	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	58		
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	58		
4	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	42		
5	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	25		



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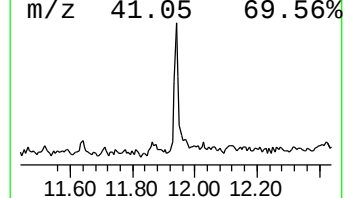
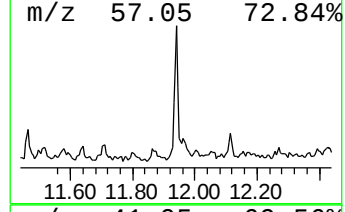
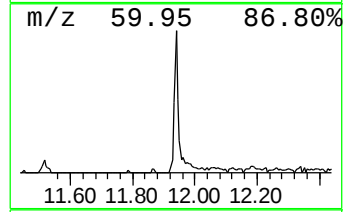
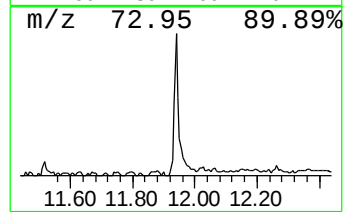
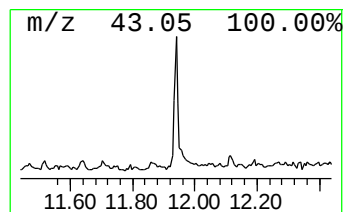
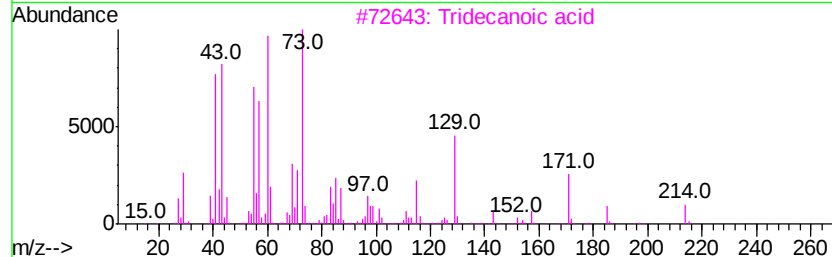
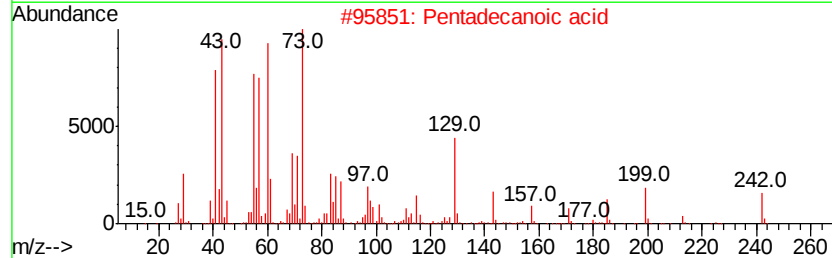
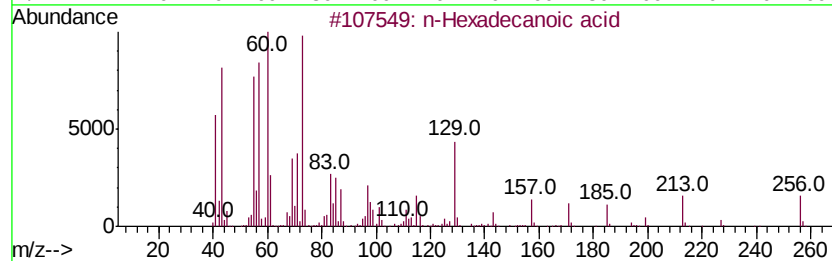
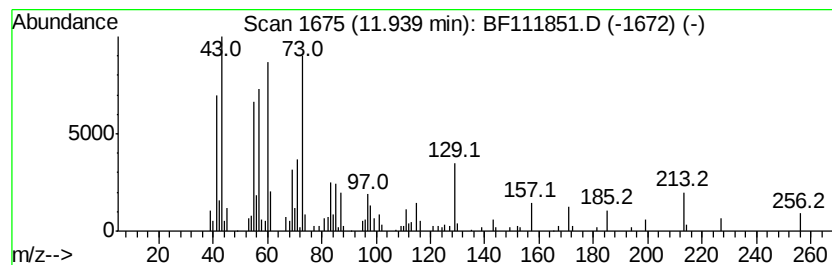
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	3.41 ng	194272	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Undecanoic acid	186	C11H22O2	000112-37-8	59
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111851.D
Acq On : 4 Jan 2019 18:14
Operator : JU/SJ
Sample : K1018-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

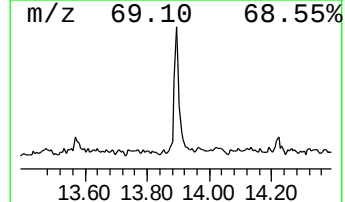
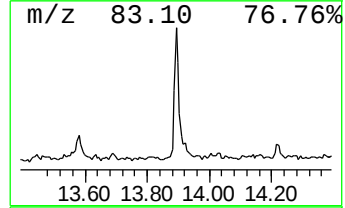
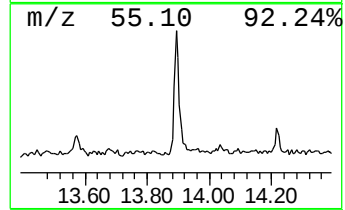
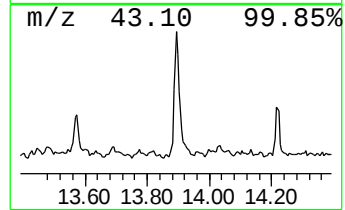
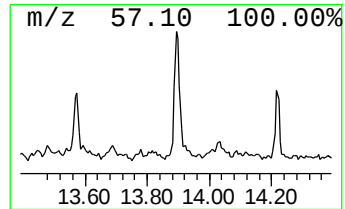
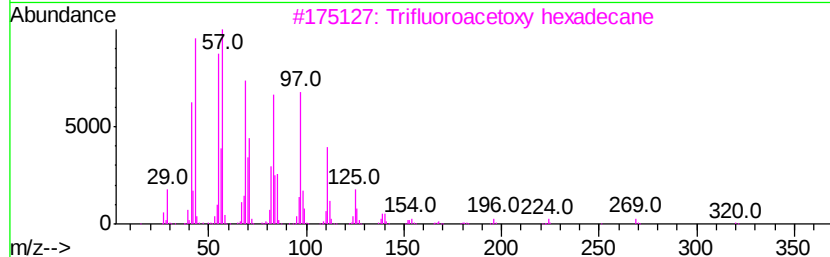
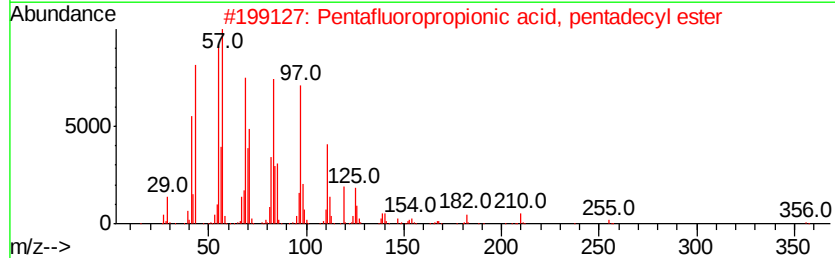
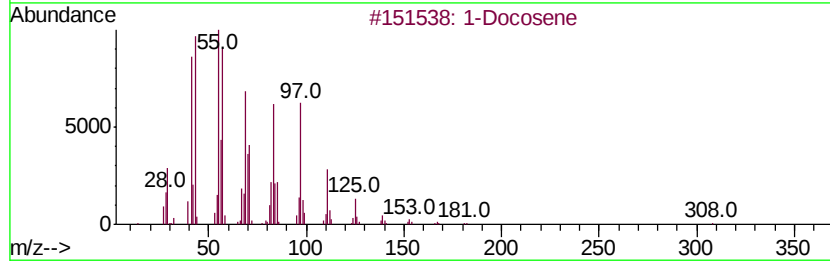
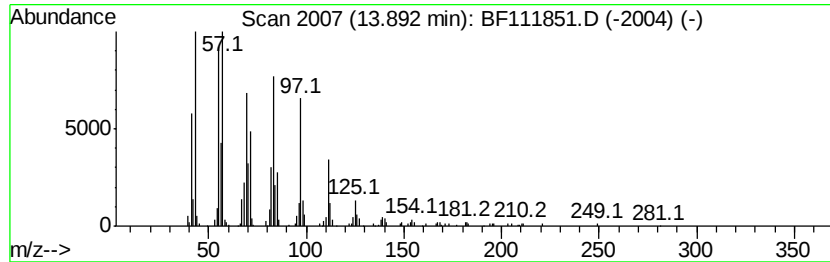
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	6.00 ng	311091	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111851.D
Acq On : 4 Jan 2019 18:14
Operator : JU/SJ
Sample : K1018-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

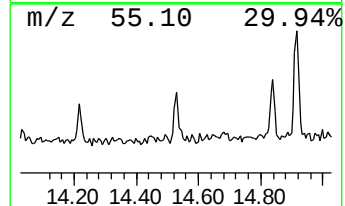
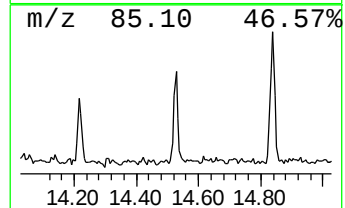
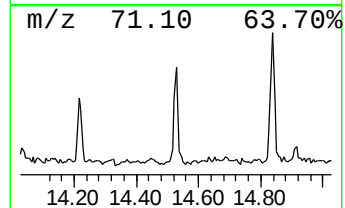
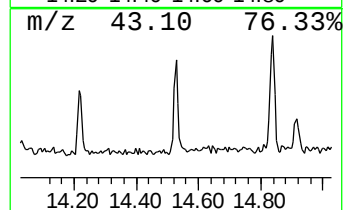
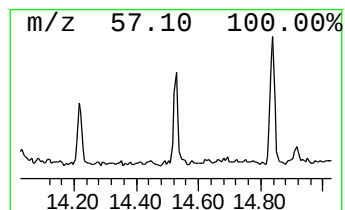
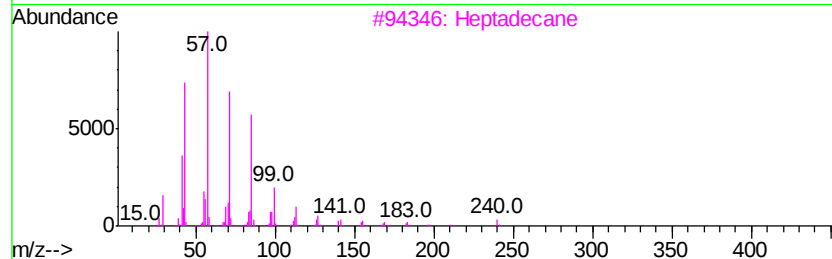
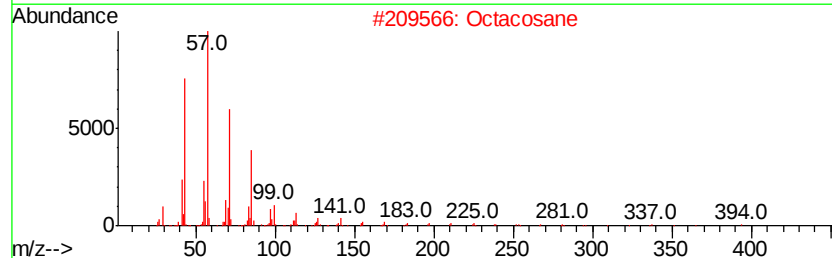
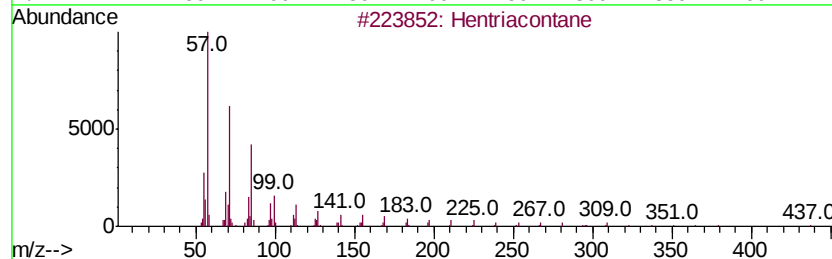
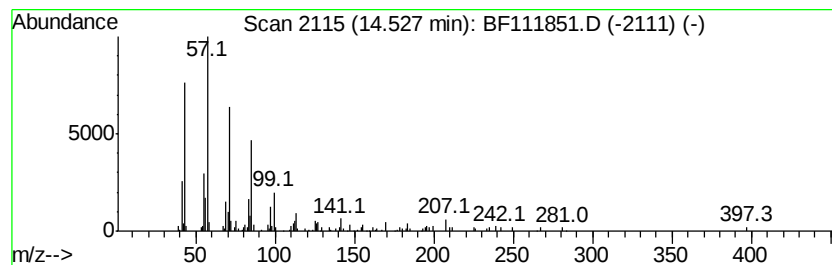
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hentriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.50 ng	129700	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	90
2	Octacosane	394	C28H58	000630-02-4	87
3	Heptadecane	240	C17H36	000629-78-7	86
4	Tetracosane	338	C24H50	000646-31-1	83
5	2-methyloctacosane	408	C29H60	1000376-72-8	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111851.D
Acq On : 4 Jan 2019 18:14
Operator : JU/SJ
Sample : K1018-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

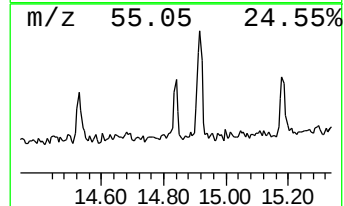
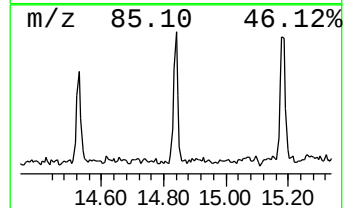
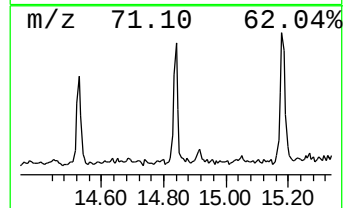
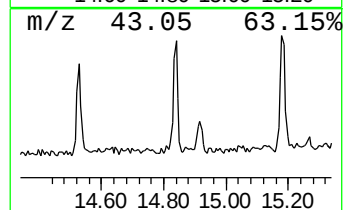
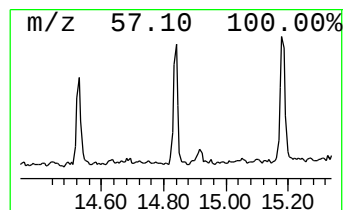
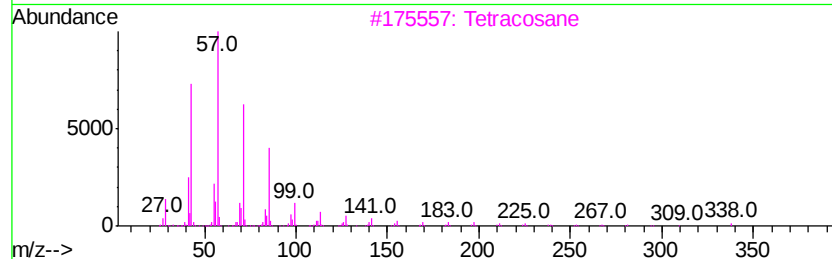
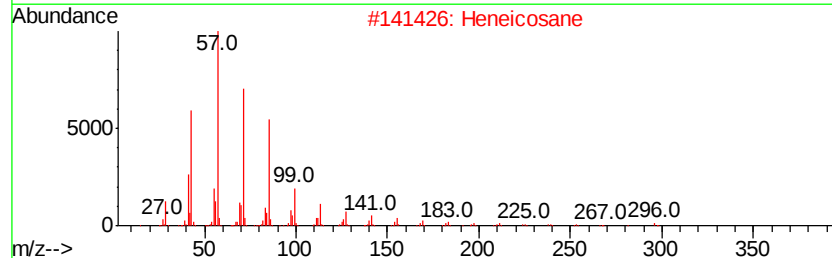
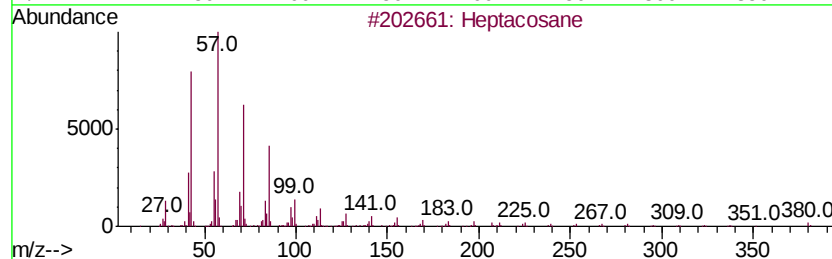
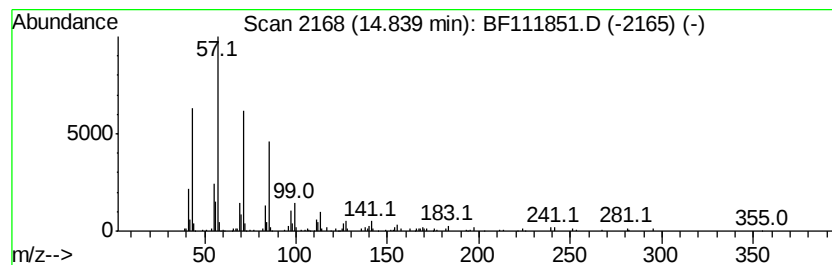
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.35 ng	140407	Perylene-d12	15.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Heneicosane	296	C21H44	000629-94-7	90
3			Tetracosane	338	C24H50	000646-31-1	90
4			2-methyloctacosane	408	C29H60	1000376-72-8	87
5			Eicosane	282	C20H42	000112-95-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111851.D
Acq On : 4 Jan 2019 18:14
Operator : JU/SJ
Sample : K1018-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

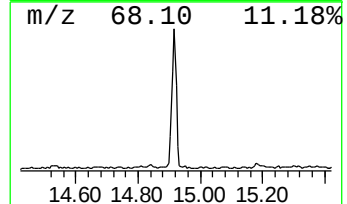
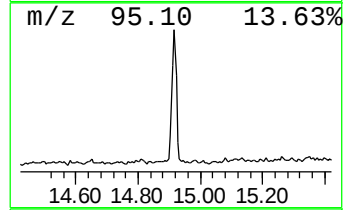
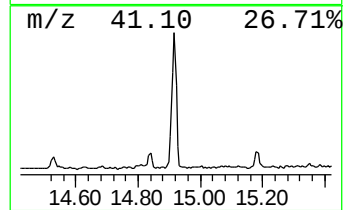
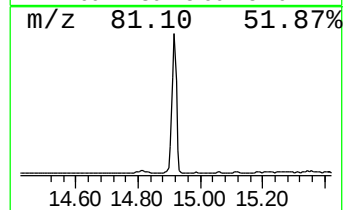
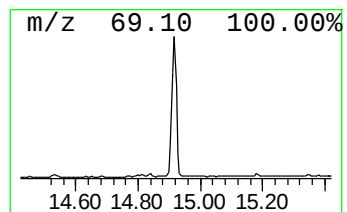
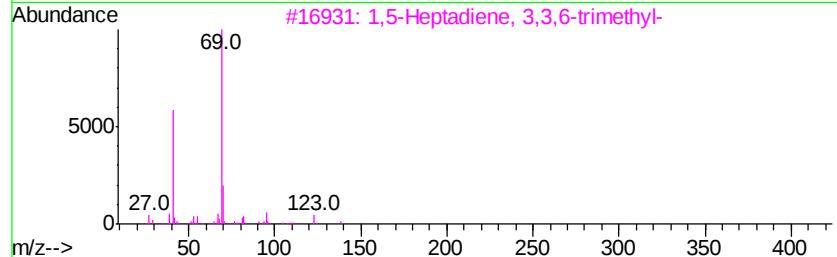
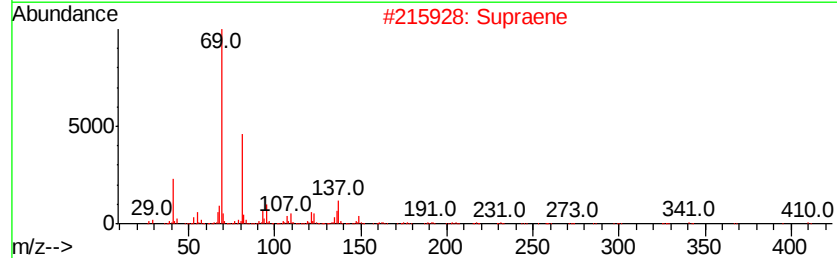
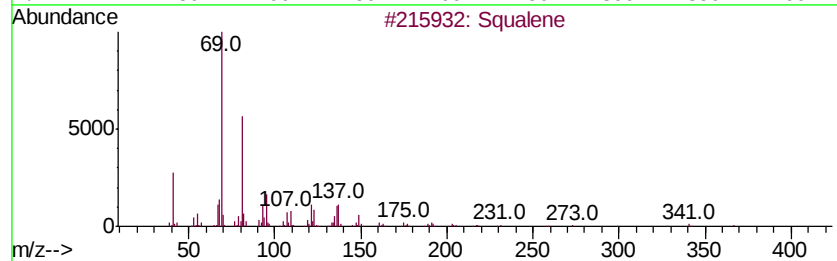
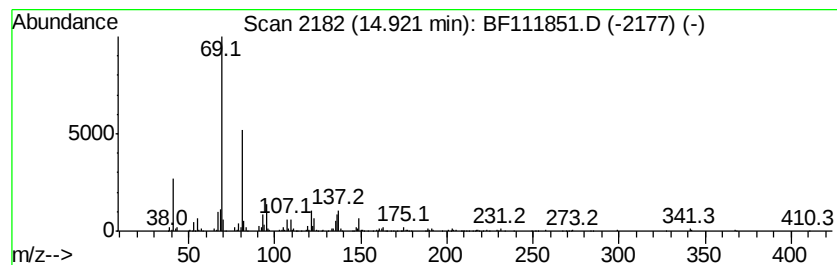
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	13.66 ng	816760	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	94
2		Supraene	410	C30H50	007683-64-9	91
3		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52
4		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50
5		2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
Data File : BF111851.D
Acq On : 4 Jan 2019 18:14
Operator : JU/SJ
Sample : K1018-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

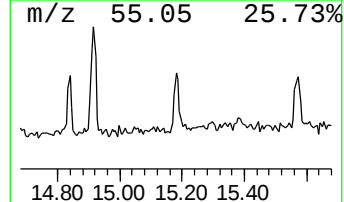
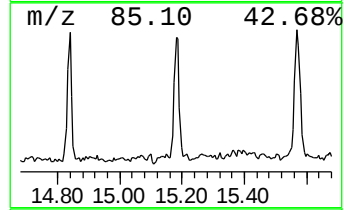
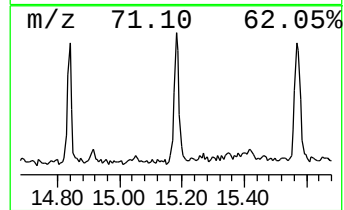
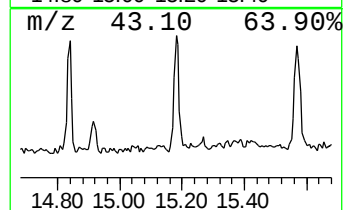
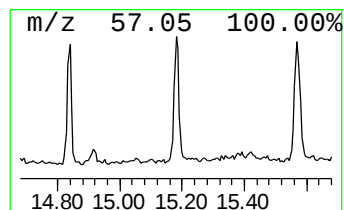
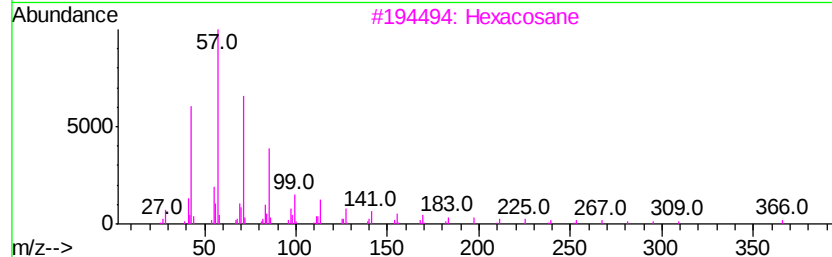
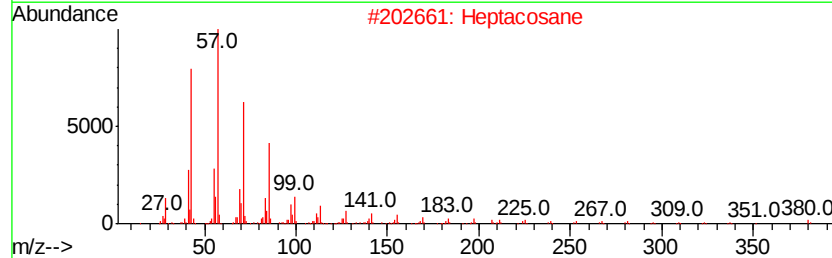
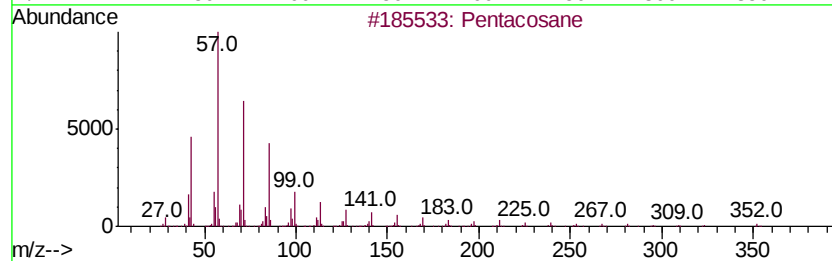
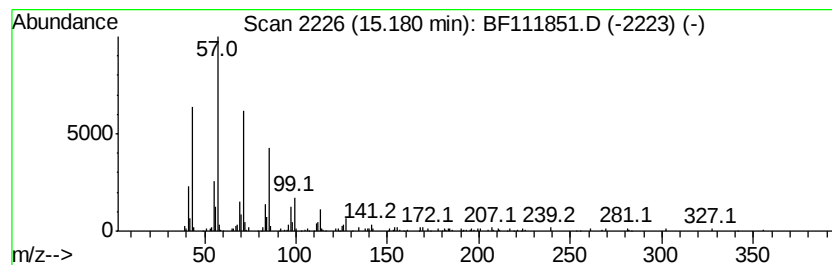
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	2.91 ng	173908	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Hexatriacontane	507	C36H74	000630-06-8	87
5		Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010419\
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Acq On : 4 Jan 2019 18:14
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Sample : K1018-02
Misc :
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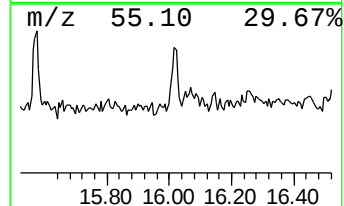
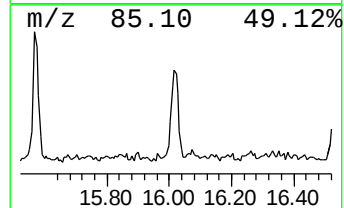
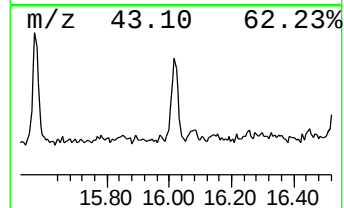
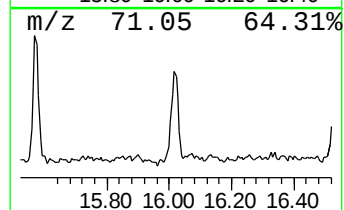
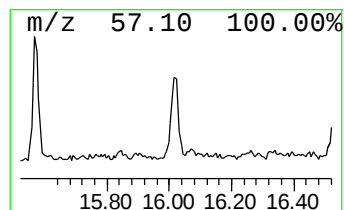
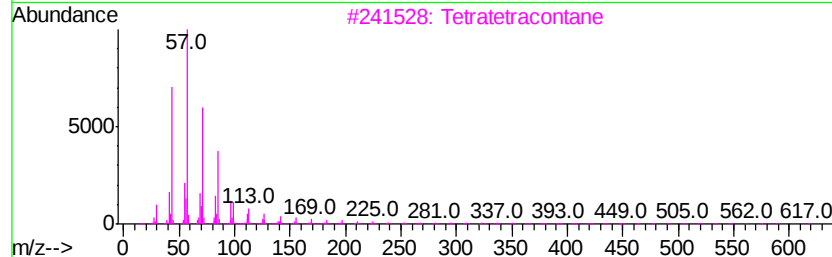
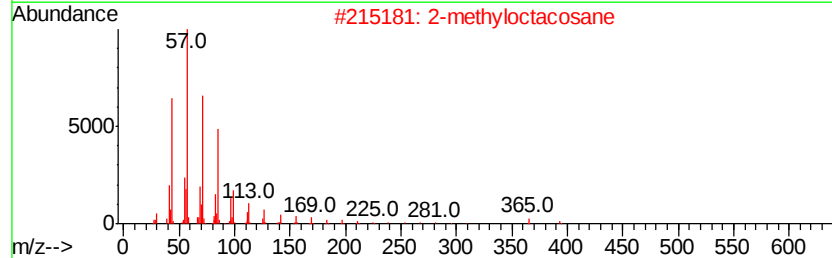
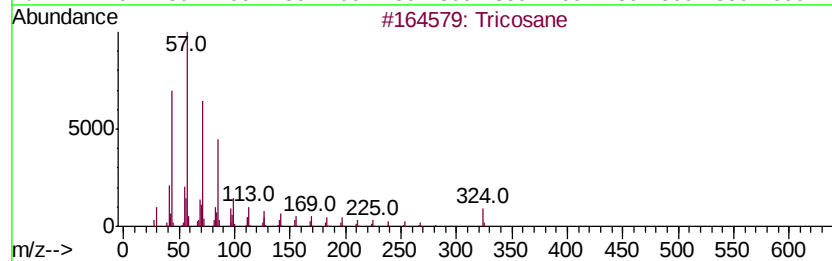
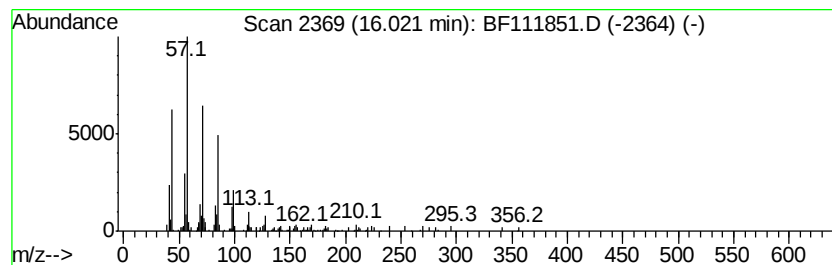
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tricosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	2.43 ng	145438	Perylene-d12	15.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosane	324	C23H48	000638-67-5	90
2			2-methyloctacosane	408	C29H60	1000376-72-8	87
3			Tetratetracontane	619	C44H90	007098-22-8	87
4			Octacosane	394	C28H58	000630-02-4	87
5			Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF010419\
 Data File : BF111851.D
 Acq On : 4 Jan 2019 18:14
 Operator : JU/SJ
 Sample : K1018-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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...	5.10	2.5	ng	133229	1	6.89	1056940	20.0
unknown6.67	6.67	73.4	ng	3879420	1	6.89	1056940	20.0
Ethanol, 2-(2-eth...	6.72	2.4	ng	127650	1	6.89	1056940	20.0
2,4,7,9-Tetrameth...	9.37	6.8	ng	475234	3	9.93	1395730	20.0
n-Hexadecanoic acid	11.94	3.4	ng	194272	4	11.42	1139090	20.0
1-Docosene	13.89	6.0	ng	311091	5	14.06	1037100	20.0
Hentriacontane	14.53	2.5	ng	129700	5	14.06	1037100	20.0
Heptacosane	14.84	2.4	ng	140407	6	15.54	1195710	20.0
Squalene	14.92	13.7	ng	816760	6	15.54	1195710	20.0
Pentacosane	15.18	2.9	ng	173908	6	15.54	1195710	20.0
Tricosane	16.02	2.4	ng	145438	6	15.54	1195710	20.0