

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122719\
 Data File : BP001467.D
 Acq On : 27 Dec 2019 19:45
 Operator : JU
 Sample : K6435-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB-4D-(21.5-23.5)

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_P\METHODS\8270-BP121919.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	5.593	591	596	614	rVB	96440	165004	12.38%	1.793%
2	6.205	694	700	716	rBV	598092	791771	59.41%	8.602%
3	7.752	956	963	977	rBV	664765	894352	67.11%	9.716%
4	7.928	987	993	1004	rBV	771121	912457	68.47%	9.913%
5	8.281	1048	1053	1063	rVB	134680	153305	11.50%	1.666%
6	8.528	1088	1095	1102	rBV	613817	749878	56.27%	8.147%
7	9.169	1197	1204	1208	rBV	462510	570358	42.80%	6.197%
8	9.798	1305	1311	1318	rBV6	6076	16127	1.21%	0.175%
9	10.316	1394	1399	1413	rBV	137594	176358	13.23%	1.916%
10	12.098	1695	1702	1719	rBV	900777	1105232	82.93%	12.008%
11	12.769	1811	1816	1830	rBV	59961	89081	6.68%	0.968%
12	13.175	1879	1885	1896	rBV	169735	225096	16.89%	2.445%
13	14.475	2098	2106	2124	rBV	553626	743549	55.79%	8.078%
14	15.575	2288	2293	2306	rVB	199201	247404	18.56%	2.688%
15	16.469	2440	2445	2453	rBV	44127	59319	4.45%	0.644%
16	17.298	2581	2586	2589	rBV	12678	15920	1.19%	0.173%
17	17.451	2603	2612	2624	rBV2	84594	141334	10.61%	1.535%
18	17.557	2627	2630	2641	rVB5	19794	35469	2.66%	0.385%
19	17.863	2676	2682	2686	rBV	1146555	1332667	100.00%	14.478%
20	18.533	2789	2796	2807	rVB	37149	52338	3.93%	0.569%
21	19.157	2895	2902	2908	rBV4	21299	65300	4.90%	0.709%
22	19.221	2908	2913	2922	rVB	215736	251773	18.89%	2.735%
23	19.898	3022	3028	3034	rBV	18750	26616	2.00%	0.289%
24	20.098	3057	3062	3072	rBV4	10164	20759	1.56%	0.226%
25	20.233	3081	3085	3088	rBV2	13018	15349	1.15%	0.167%
26	20.268	3088	3091	3096	rVB2	19806	24828	1.86%	0.270%
27	20.663	3154	3158	3163	rVB2	19580	24296	1.82%	0.264%
28	20.986	3207	3213	3222	rBV2	145589	206845	15.52%	2.247%
29	21.092	3227	3231	3238	rVB2	17497	25766	1.93%	0.280%
30	21.586	3309	3315	3320	rBV2	14613	25580	1.92%	0.278%
31	21.727	3330	3339	3340	rBV9	10668	22573	1.69%	0.245%
32	22.145	3405	3410	3419	rVB3	8164	17801	1.34%	0.193%

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Instrument :
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ClientSampleId :
SB-4D-(21.5-23.5)

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_P\METHODS\8270-BP121919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

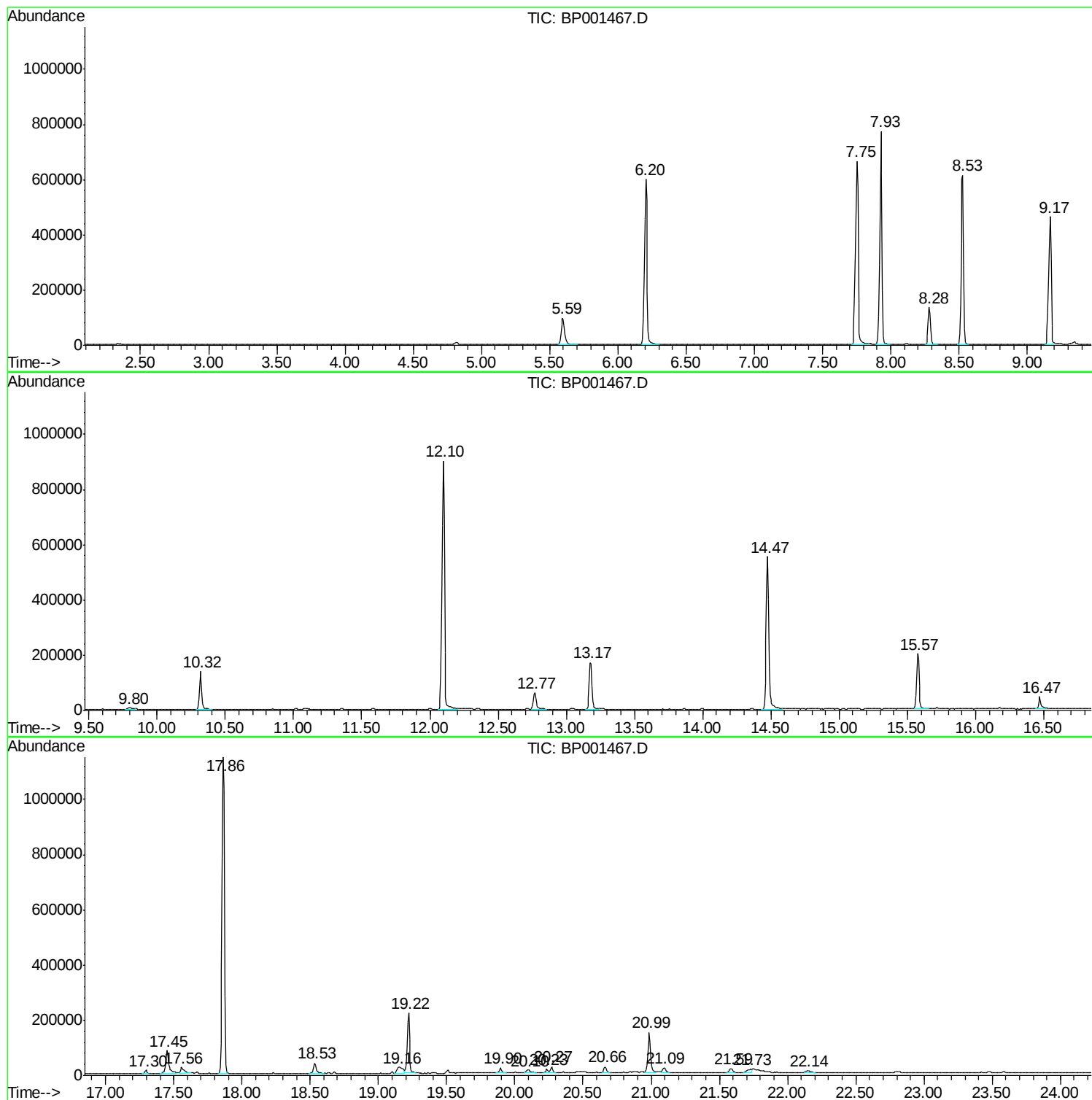
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP121919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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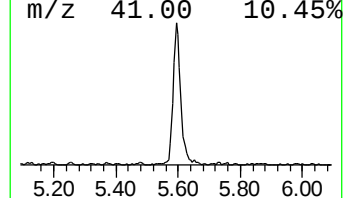
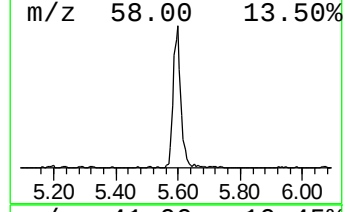
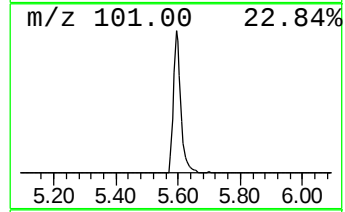
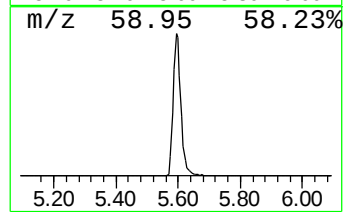
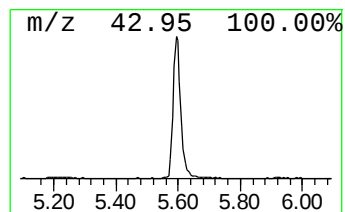
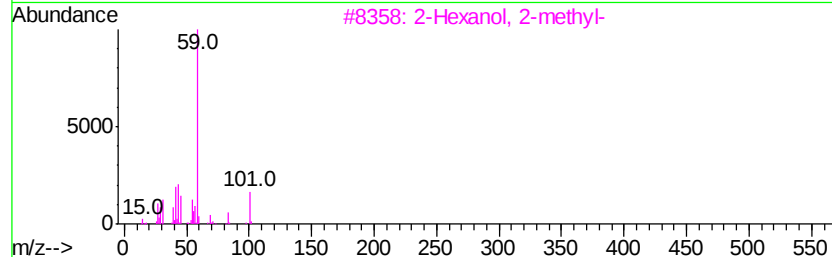
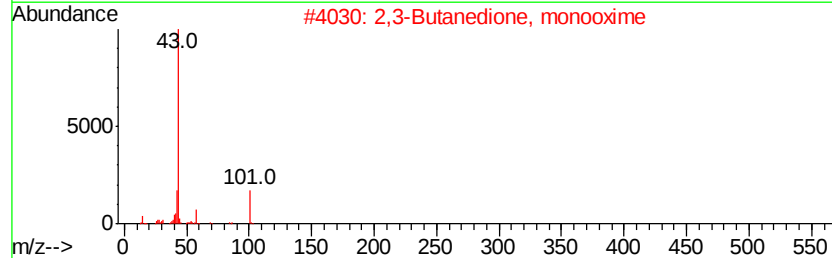
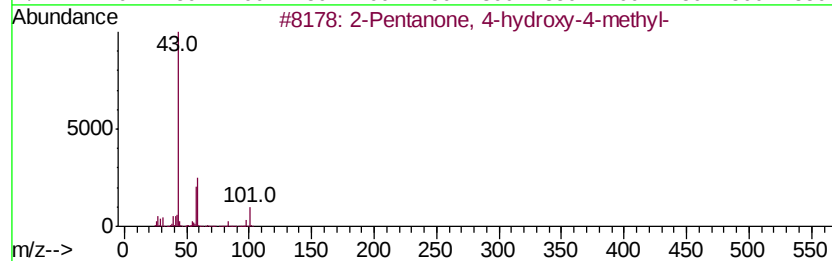
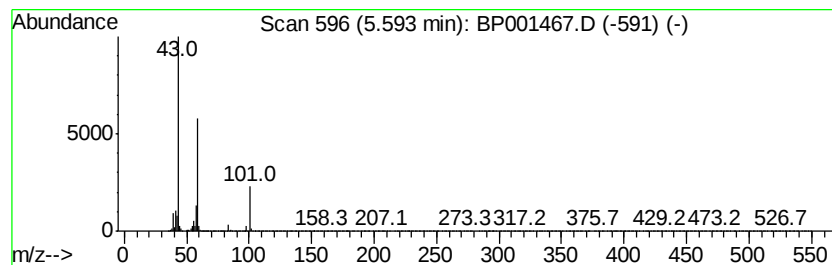
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.59	21.53 ng	165004	1,4-Dichlorobenzene-d4	8.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	17
5			Butane	58	C4H10	000106-97-8	14



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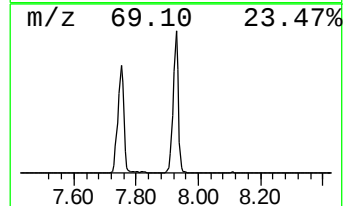
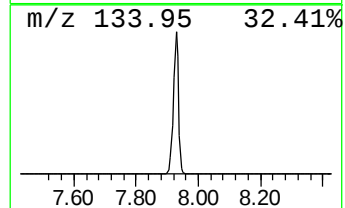
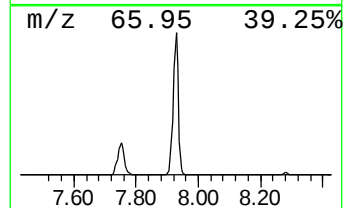
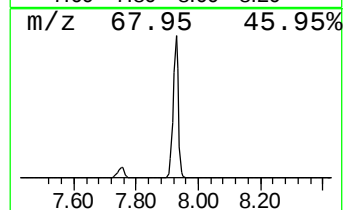
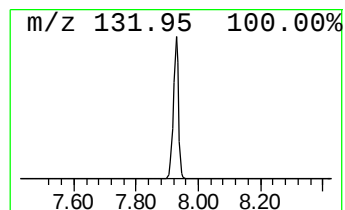
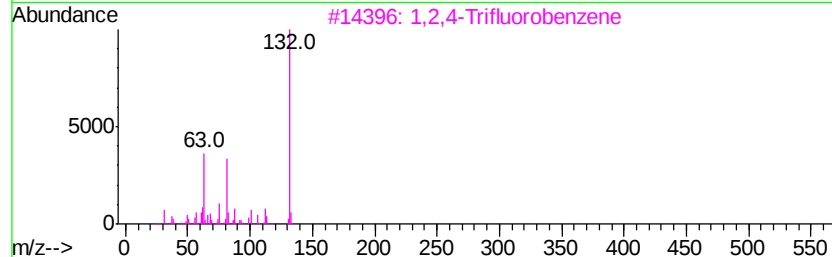
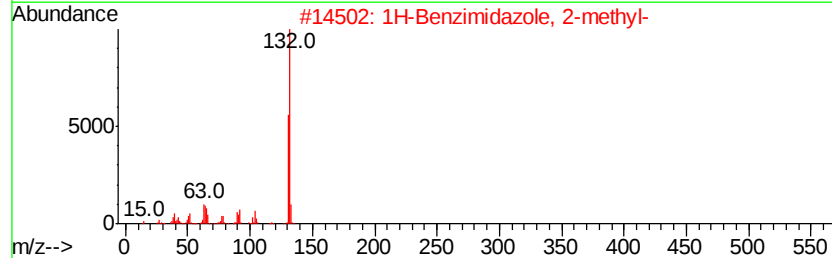
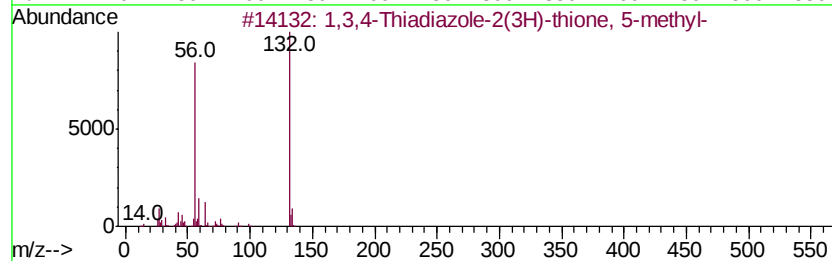
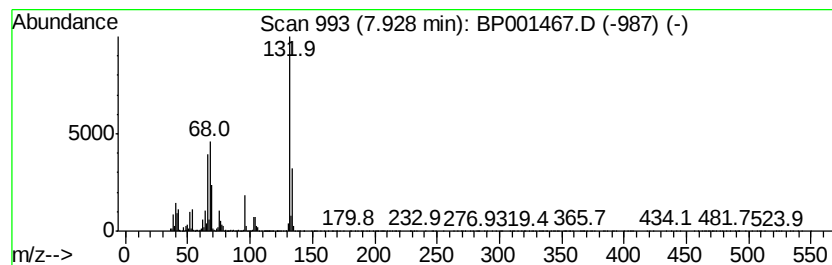
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.93 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.93	119.04 ng	912457	1,4-Dichlorobenzene-d4	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
3		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10



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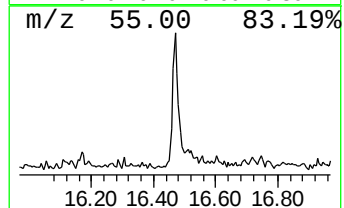
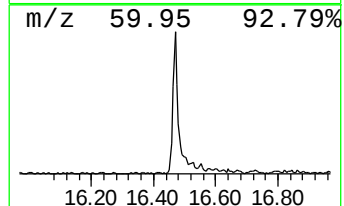
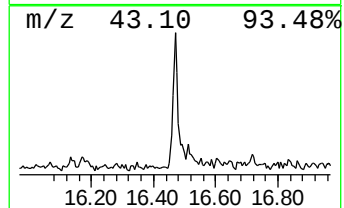
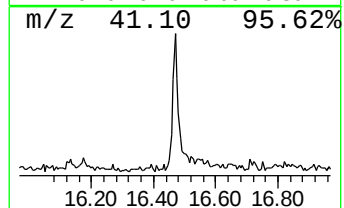
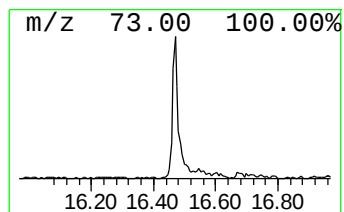
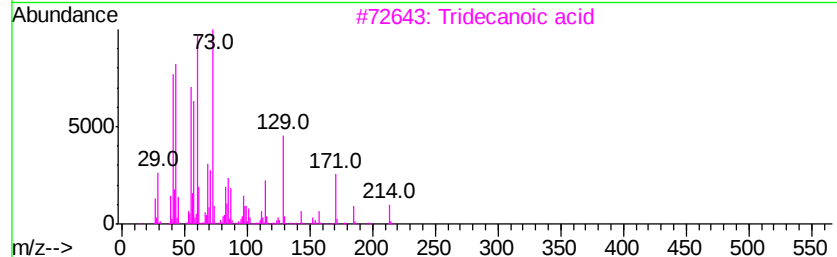
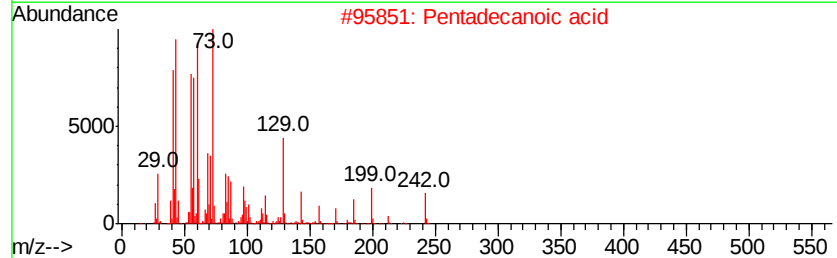
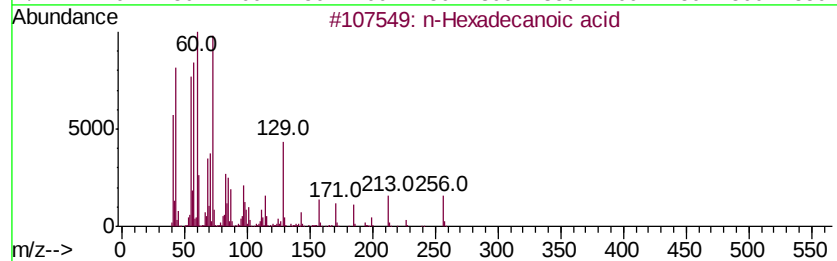
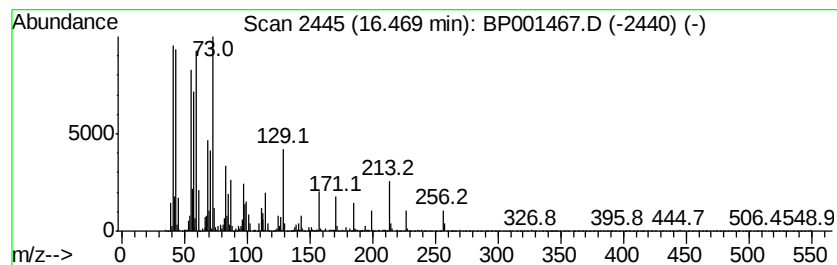
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	4.80 ng	59319	Phenanthrene-d10	15.57

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3		Tridecanoic acid	214	C13H26O2	000638-53-9	70
4		n-Decanoic acid	172	C10H20O2	000334-48-5	68
5		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53



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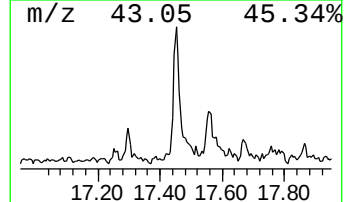
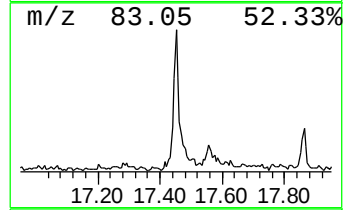
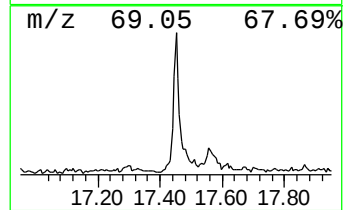
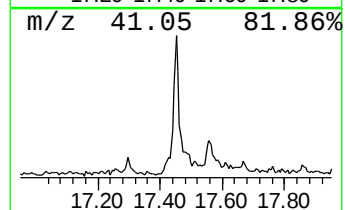
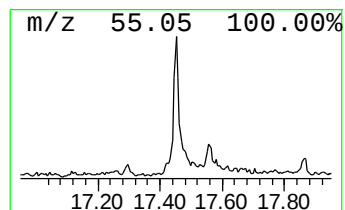
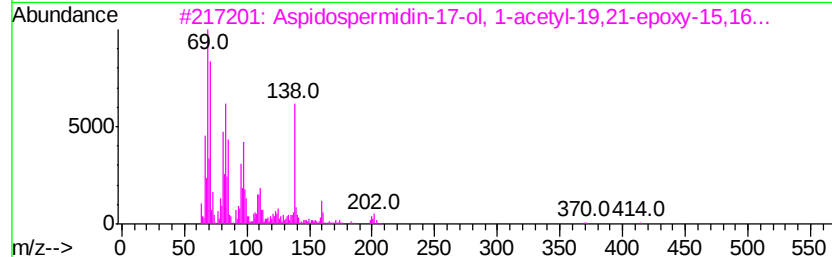
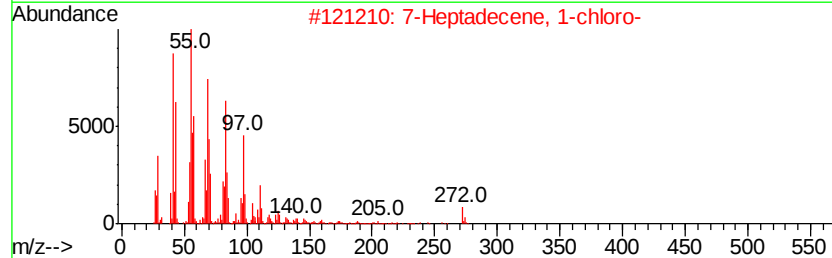
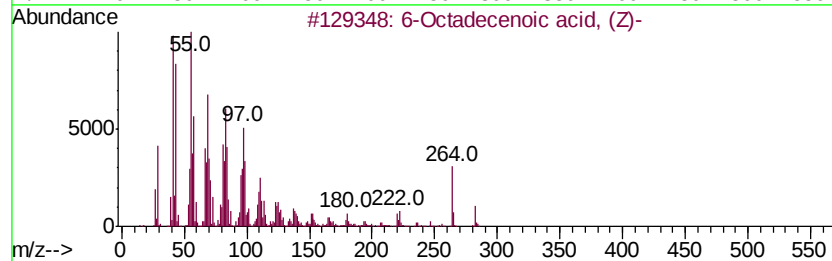
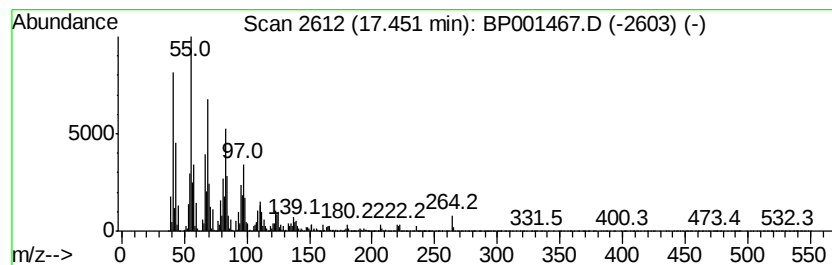
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ClientSampleID :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 6-Octadecenoic acid, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.45	11.23 ng	141334	Chrysene-d12	19.22		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	87
2		7-Heptadecene, 1-chloro-	272	C17H33Cl	056554-78-0	76
3		Aspidospermidin-17-ol, 1-acetyl-...	414	C23H30N2O5	002122-26-1	76
4		cis-Vaccenic acid	282	C18H34O2	000506-17-2	76
5		9-octadecanoic acid, 2,2,3,3,4,4...	464	C22H35F7O2	1000376-61-4	70



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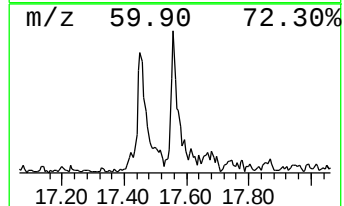
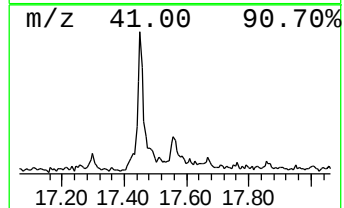
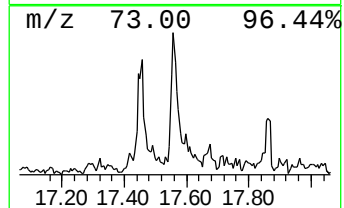
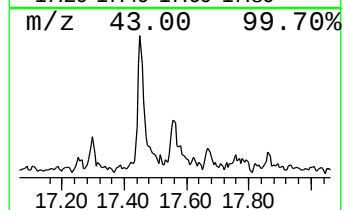
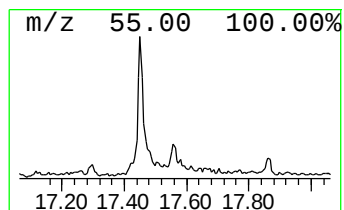
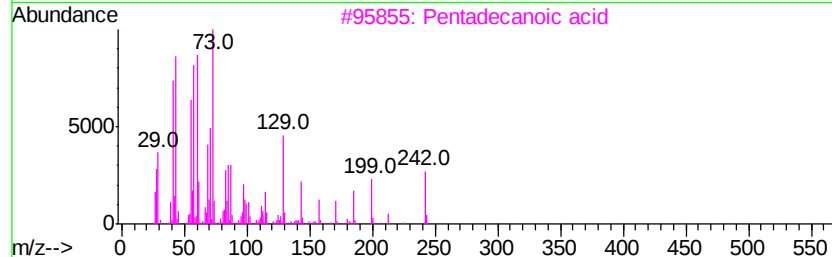
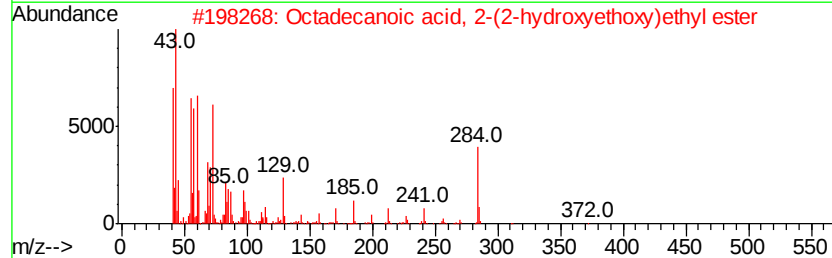
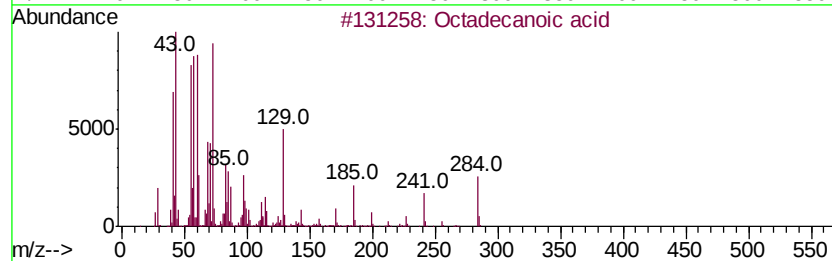
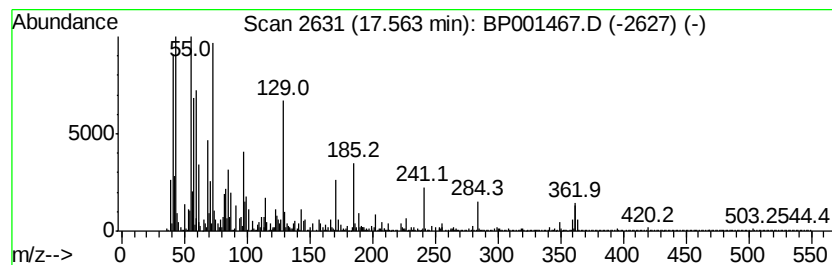
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.56	2.82 ng	35469	Chrysene-d12	19.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	83
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64



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Data File : BP001467.D
Acq On : 27 Dec 2019 19:45
Operator : JU
Sample : K6435-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

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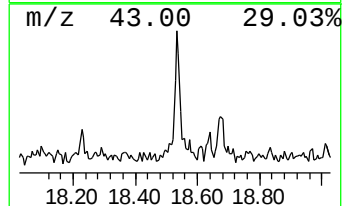
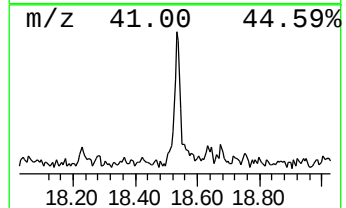
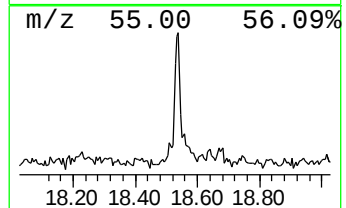
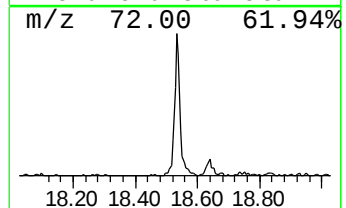
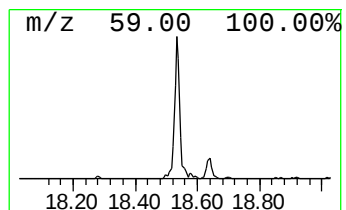
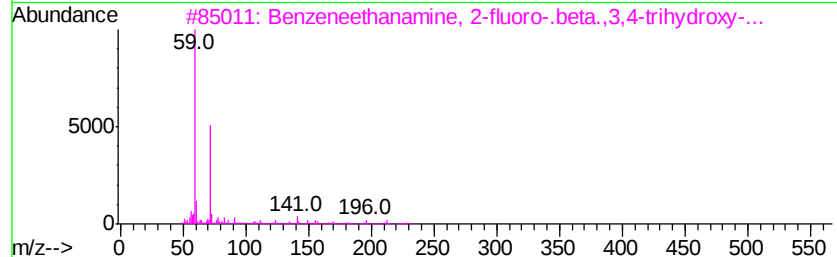
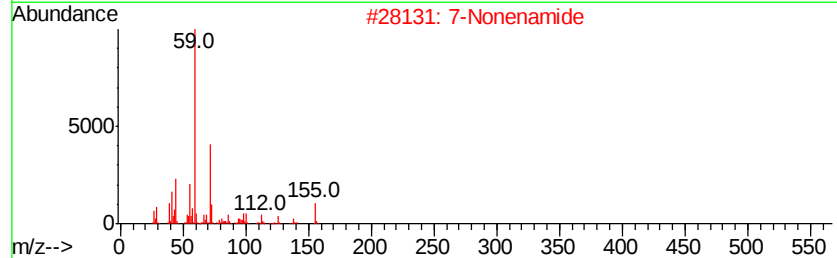
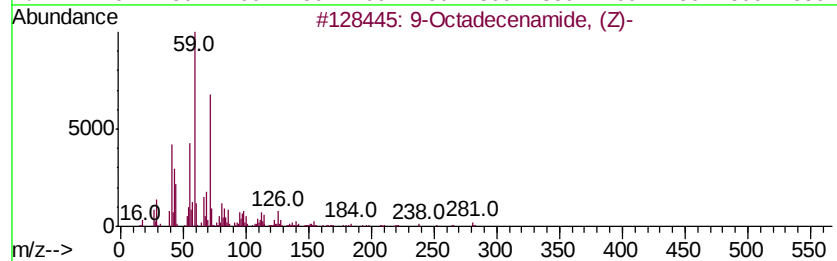
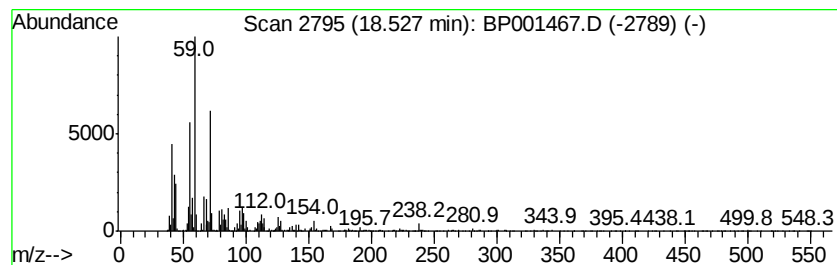
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.53	4.16 ng	52338	Chrysene-d12	19.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2		7-Nonenamide	155	C9H17NO	090949-53-4	64
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	59
5		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122719\
Data File : BP001467.D
Acq On : 27 Dec 2019 19:45
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Misc :
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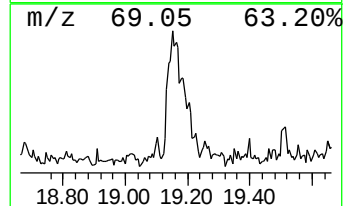
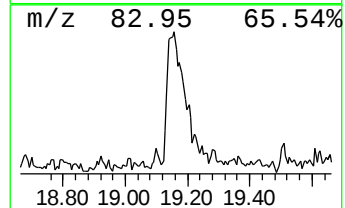
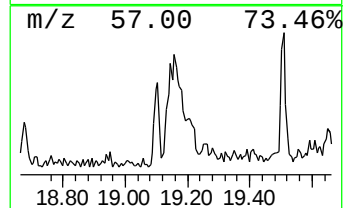
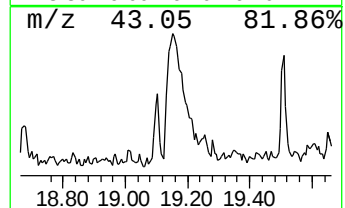
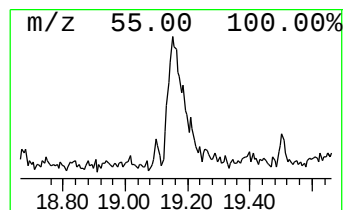
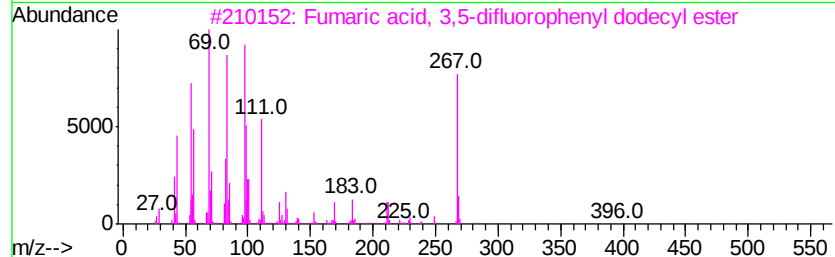
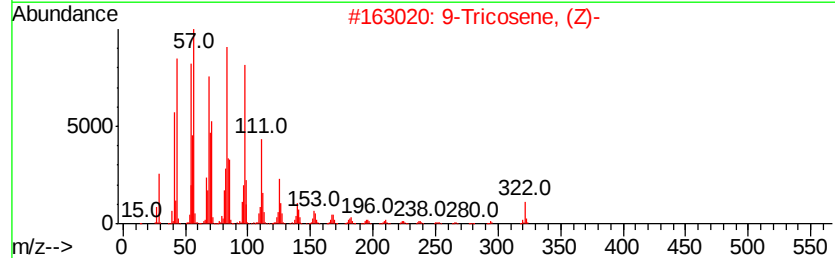
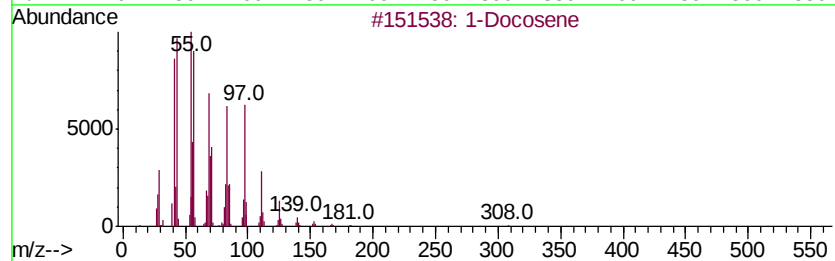
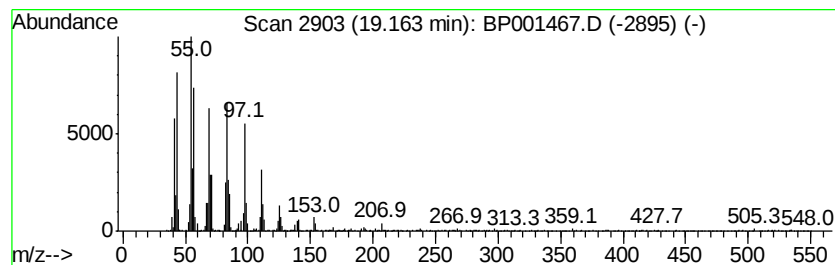
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.16	5.19 ng	65300	Chrysene-d12	19.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	95
2		9-Tricosene, (Z)-	322	C23H46	027519-02-4	91
3		Fumaric acid, 3,5-difluorophenyl...	396	C22H30F2O4	1000339-37-8	87
4		1-Tetradecene	196	C14H28	001120-36-1	83
5		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122719\
Data File : BP001467.D
Acq On : 27 Dec 2019 19:45
Operator : JU
Sample : K6435-01
Misc :
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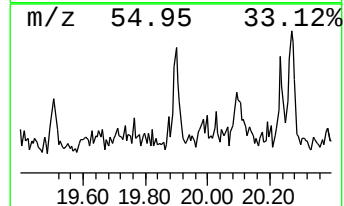
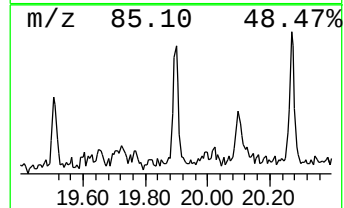
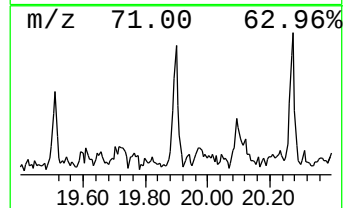
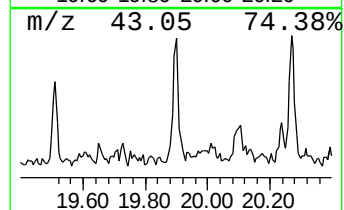
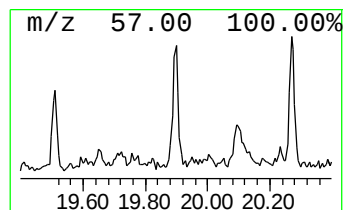
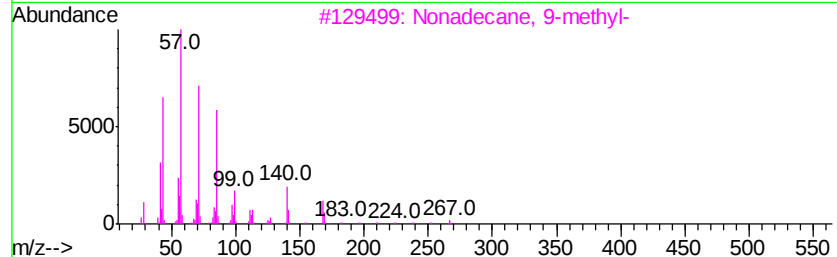
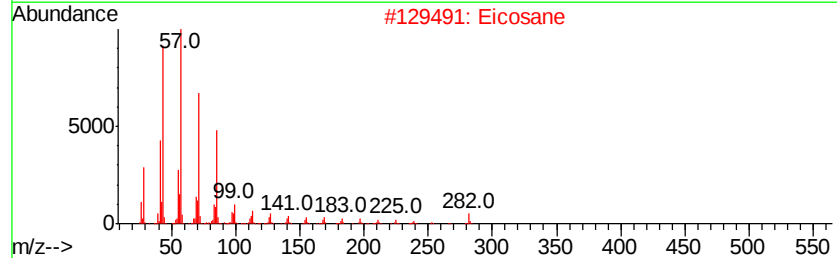
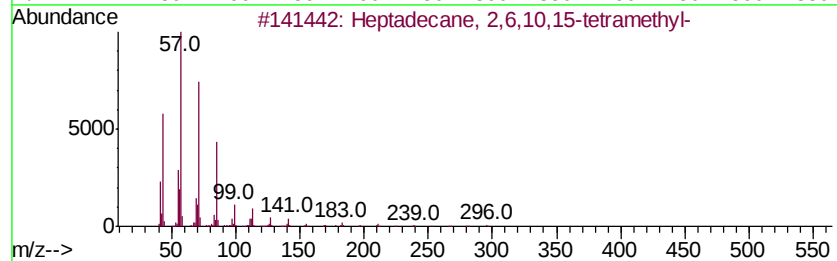
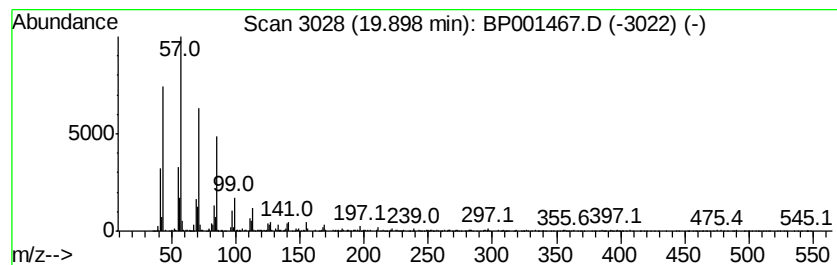
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane, 2,6,10,15-tetr... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	2.11 ng	26616	Chrysene-d12	19.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	97
2		Eicosane	282	C20H42	000112-95-8	93
3		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
4		Heneicosane	296	C21H44	000629-94-7	93
5		Docosane	310	C22H46	000629-97-0	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122719\
Data File : BP001467.D
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Operator : JU
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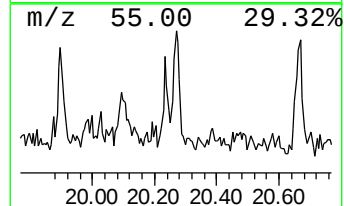
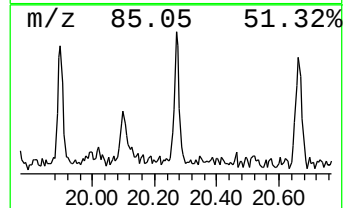
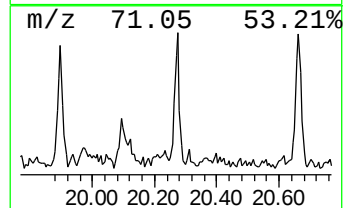
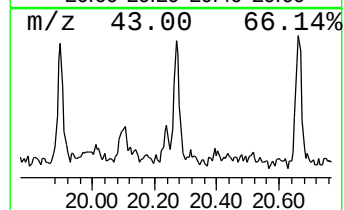
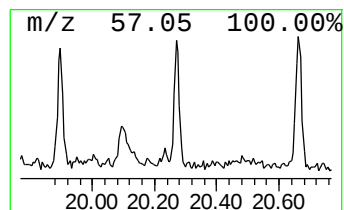
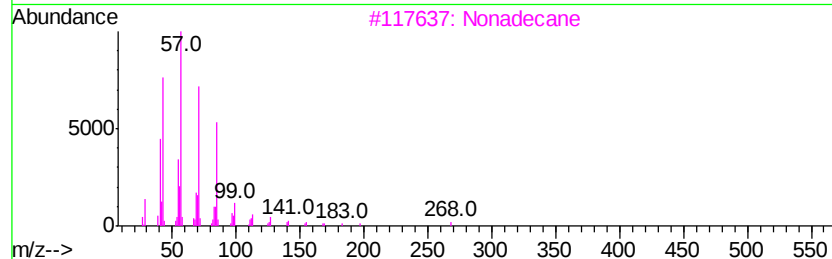
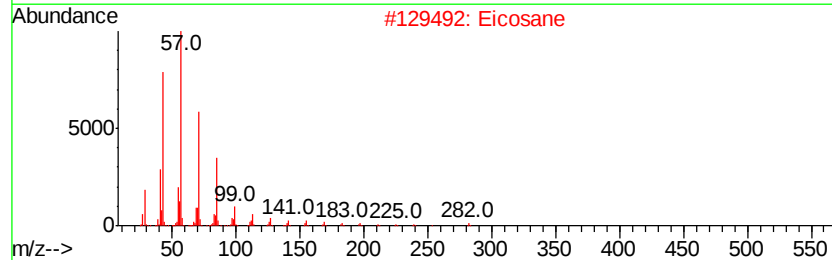
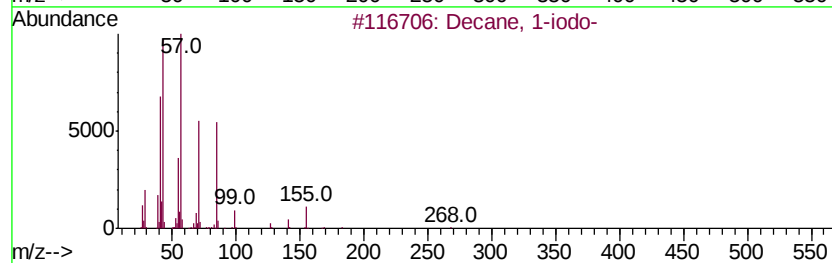
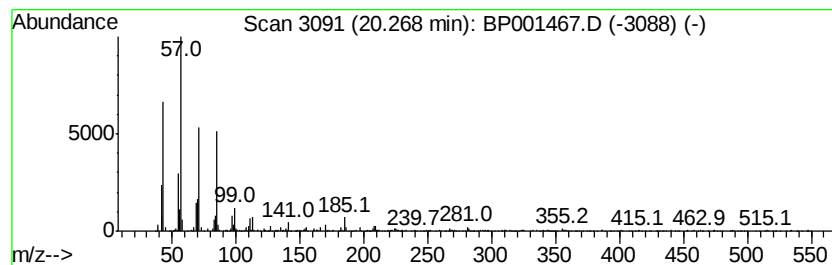
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Decane, 1-iodo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.27	2.40 ng	24828	Perylene-d12	20.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 1-iodo-	268	C10H21I	002050-77-3	87
2		Eicosane	282	C20H42	000112-95-8	86
3		Nonadecane	268	C19H40	000629-92-5	80
4		Pentadecane	212	C15H32	000629-62-9	80
5		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122719\
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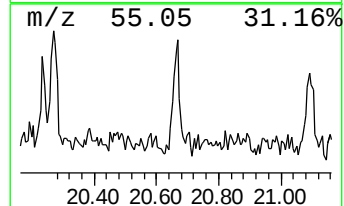
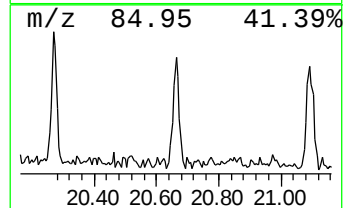
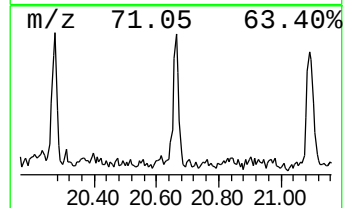
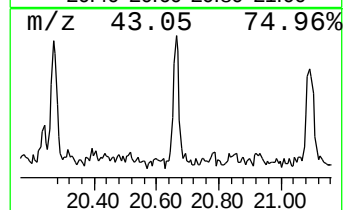
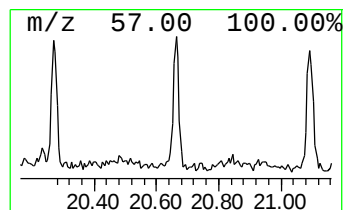
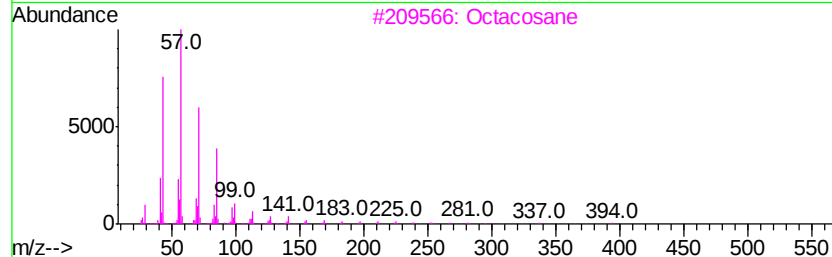
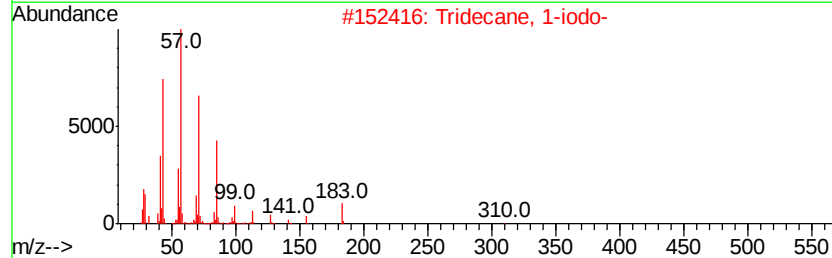
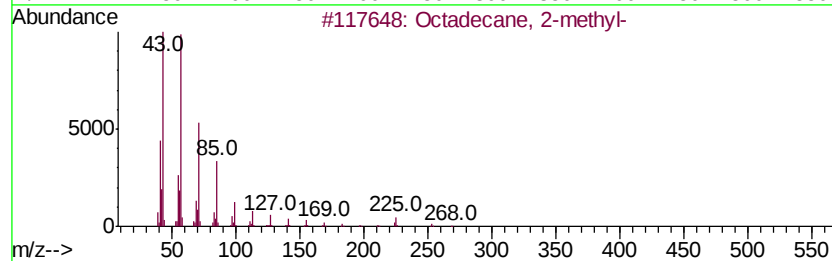
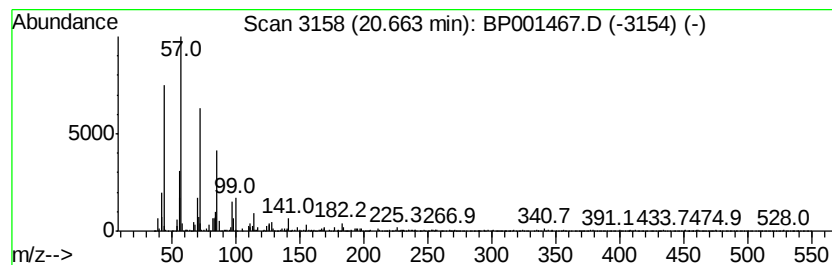
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Octadecane, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.66	2.35 ng	24296	Perylene-d12	20.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
3		Octacosane	394	C28H58	000630-02-4	90
4		Heptacosane	380	C27H56	000593-49-7	87
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122719\
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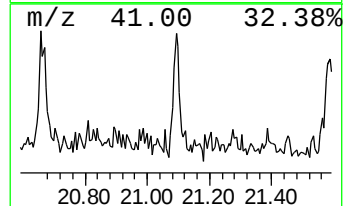
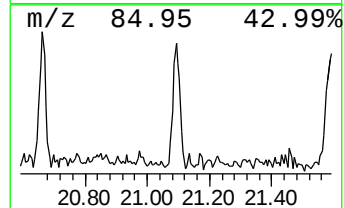
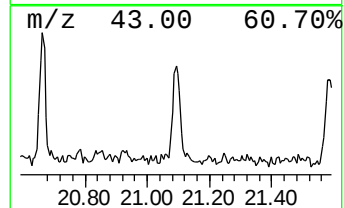
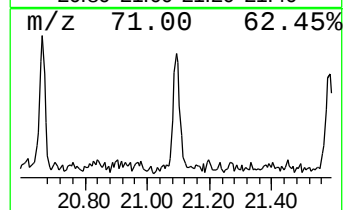
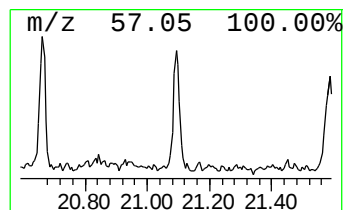
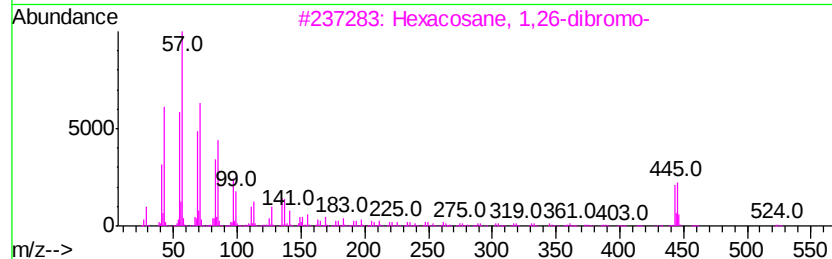
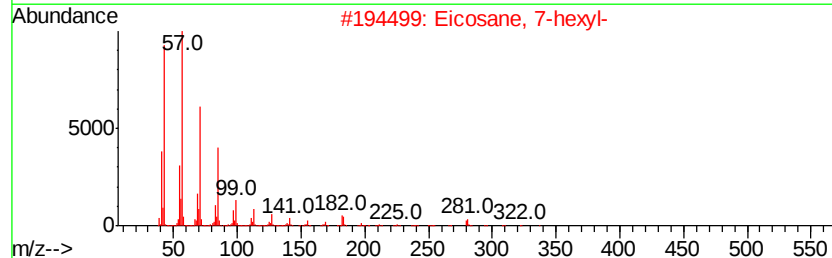
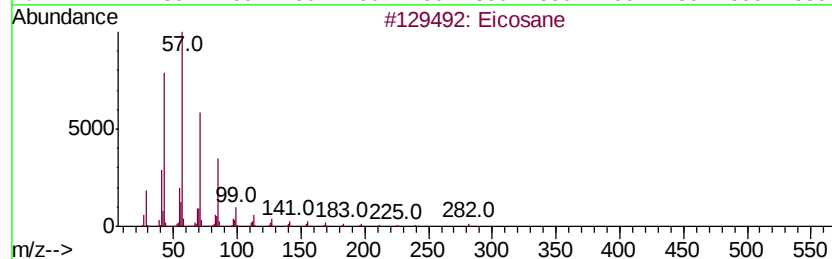
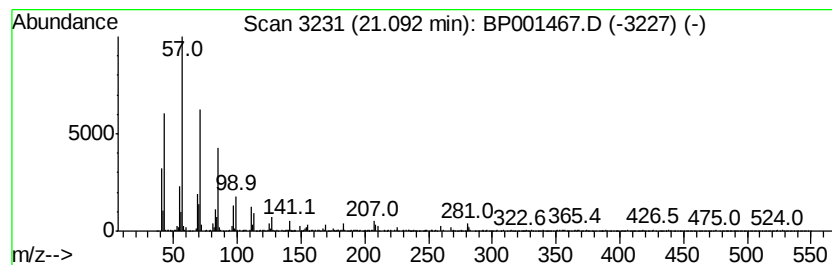
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.09	2.49 ng	25766	Perylene-d12	20.99

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	90
2	Eicosane, 7-hexyl-			366	C26H54	055333-99-8	83
3	Hexacosane, 1,26-dibromo-			522	C26H52Br2	143389-26-8	83
4	Hexacosane			366	C26H54	000630-01-3	81
5	Docosane, 11-decyl-			451	C32H66	055401-55-3	81



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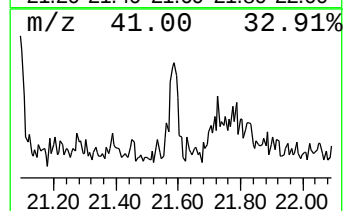
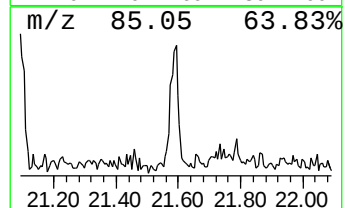
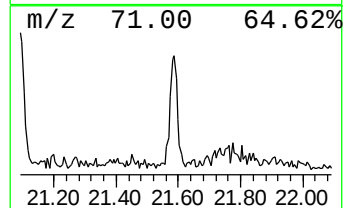
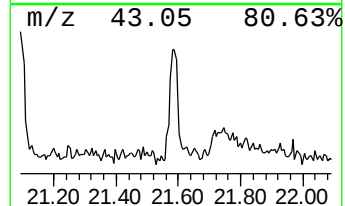
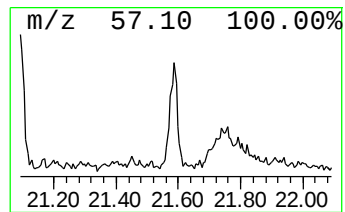
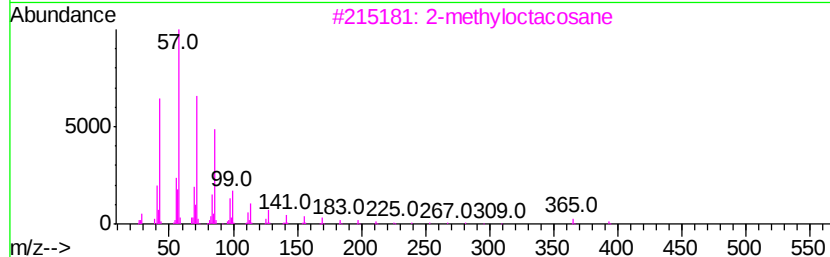
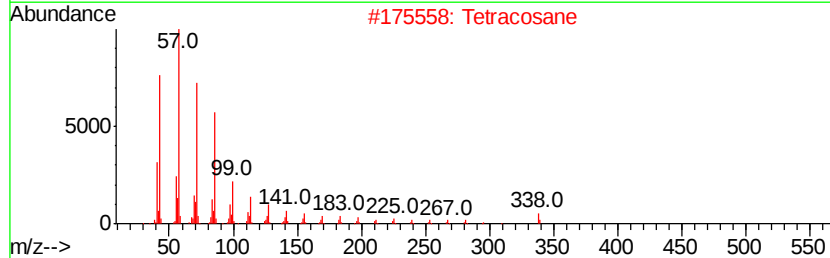
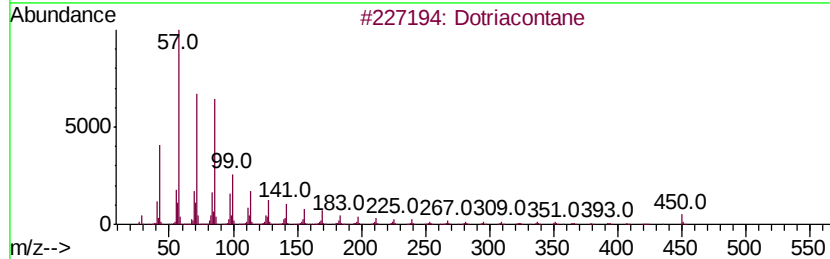
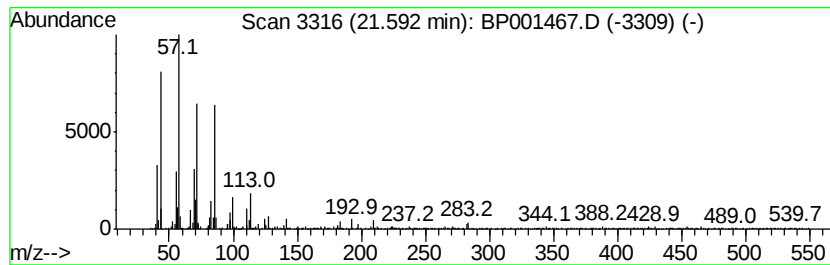
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Dotriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.59	2.47 ng	25580	Perylene-d12	20.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dotriacontane	451	C32H66	000544-85-4	94
2		Tetracosane	338	C24H50	000646-31-1	86
3		2-methyloctacosane	408	C29H60	1000376-72-8	83
4		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	80
5		Hexacosane	366	C26H54	000630-01-3	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122719\
Data File : BP001467.D
Acq On : 27 Dec 2019 19:45
Operator : JU
Sample : K6435-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-4D-(21.5-23.5)

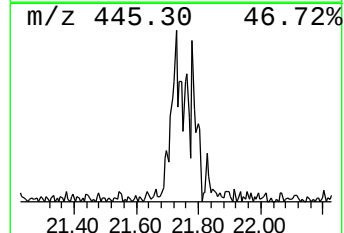
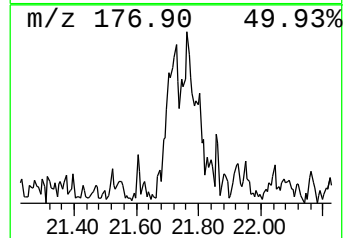
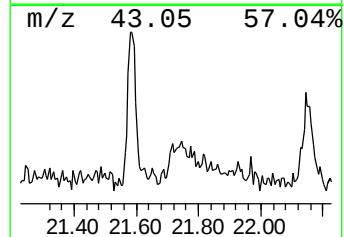
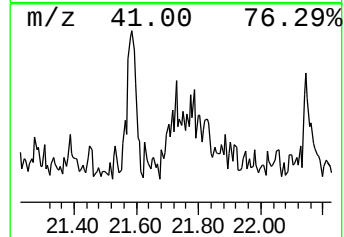
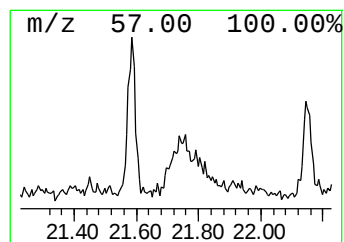
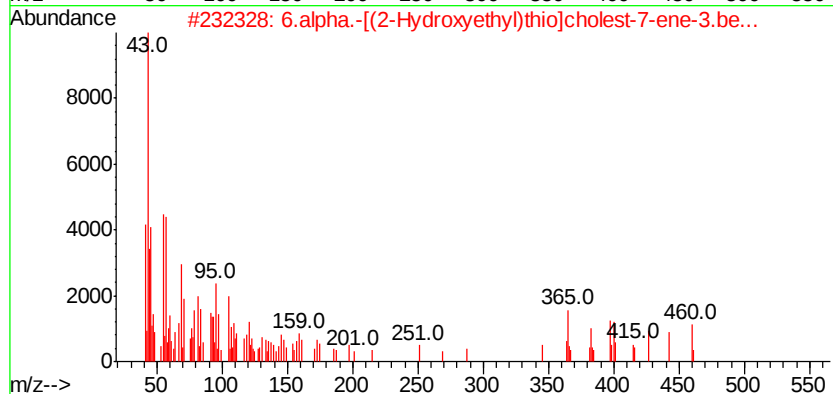
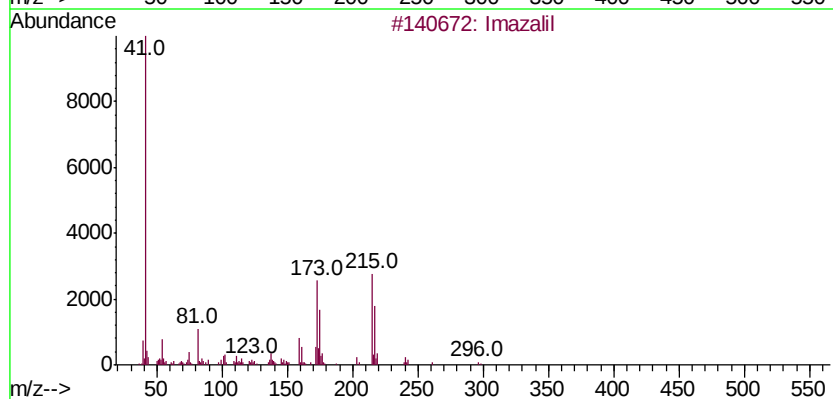
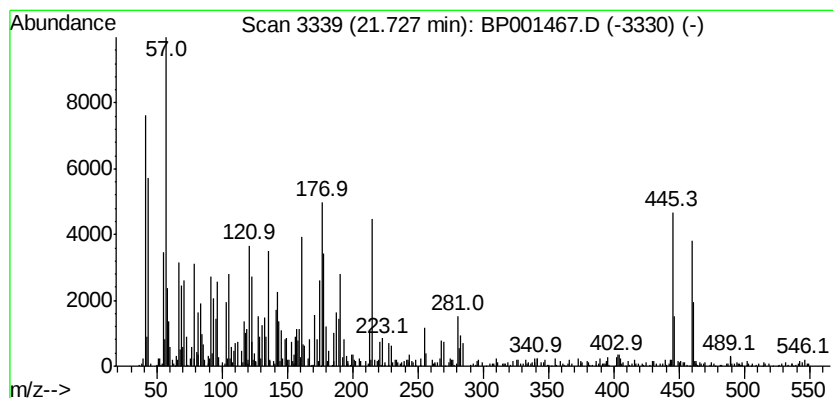
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown21.73 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.73	2.18 ng	22573	Perylene-d12	20.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	2	Imazalil	296	C14H14Cl2N2O	035554-44-0	9
2		6.alpha.-(2-Hydroxyethyl)thio]c...	478	C29H50O3S	095841-74-0	1



Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP122719\
 Data File : BP001467.D
 Acq On : 27 Dec 2019 19:45
 Operator : JU
 Sample : K6435-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB-4D-(21.5-23.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.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
2-Pentanone, 4-hy...	5.59	21.5	ng	165004	1	8.28	153305	20.0
unknown7.93	7.93	119.0	ng	912457	1	8.28	153305	20.0
n-Hexadecanoic acid	16.47	4.8	ng	59319	4	15.57	247404	20.0
6-Octadecenoic ac...	17.45	11.2	ng	141334	5	19.22	251773	20.0
Octadecanoic acid	17.56	2.8	ng	35469	5	19.22	251773	20.0
9-Octadecenamide,...	18.53	4.2	ng	52338	5	19.22	251773	20.0
1-Docosene	19.16	5.2	ng	65300	5	19.22	251773	20.0
Heptadecane, 2,6,...	19.90	2.1	ng	26616	5	19.22	251773	20.0
Decane, 1-iodo-	20.27	2.4	ng	24828	6	20.99	206845	20.0
Octadecane, 2-met...	20.66	2.4	ng	24296	6	20.99	206845	20.0
Eicosane	21.09	2.5	ng	25766	6	20.99	206845	20.0
Dotriacontane	21.59	2.5	ng	25580	6	20.99	206845	20.0
unknown21.73	21.73	2.2	ng	22573	6	20.99	206845	20.0