

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
 Data File : BF138295.D
 Acq On : 21 Jun 2024 20:06
 Operator : CG\JU
 Sample : P2977-06
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OSTL-A6

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-BF061224.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138295.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	10	15	21	rVB	2394687	2917914	56.90%	7.264%
2	3.387	219	221	237	rBV	51230	109245	2.13%	0.272%
3	5.104	509	513	520	rVB	231737	279492	5.45%	0.696%
4	5.504	576	581	584	rBV	4572910	4216473	82.22%	10.496%
5	5.828	633	636	644	rBV	79499	69461	1.35%	0.173%
6	6.510	747	752	755	rBV	4379932	4175023	81.41%	10.393%
7	6.881	812	815	819	rBV	1854342	1529585	29.83%	3.808%
8	7.445	906	911	914	rBV	3091947	2716725	52.98%	6.763%
9	7.692	950	953	957	rBV	163029	135873	2.65%	0.338%
10	8.163	1029	1033	1036	rBV	2574722	1974081	38.50%	4.914%
11	8.475	1082	1086	1098	rBV	179876	200733	3.91%	0.500%
12	9.239	1212	1216	1219	rBV	6165724	5128081	100.00%	12.766%
13	9.916	1328	1331	1335	rBV	2436195	2036655	39.72%	5.070%
14	10.016	1343	1348	1351	rBV	54614	69868	1.36%	0.174%
15	10.704	1461	1465	1468	rBV	2900517	2405793	46.91%	5.989%
16	11.404	1580	1584	1587	rBV	1827687	1564625	30.51%	3.895%
17	11.927	1670	1673	1686	rVB	487965	442646	8.63%	1.102%
18	12.616	1786	1790	1792	rBV	138211	133889	2.61%	0.333%
19	12.710	1803	1806	1814	rBV2	91723	107293	2.09%	0.267%
20	12.839	1823	1828	1831	rBV	114780	115578	2.25%	0.288%
21	12.986	1849	1853	1857	rBV	4277102	3663460	71.44%	9.120%
22	13.892	2003	2007	2012	rBV2	146670	260862	5.09%	0.649%
23	14.039	2028	2032	2035	rBV	1768823	1536221	29.96%	3.824%
24	14.510	2109	2112	2114	rBV	78165	78819	1.54%	0.196%
25	14.898	2174	2178	2182	rBV	529162	514184	10.03%	1.280%
26	14.968	2186	2190	2199	rBV	431635	444338	8.66%	1.106%
27	15.080	2205	2209	2212	rBV	71962	103975	2.03%	0.259%
28	15.163	2219	2223	2226	rBV	128081	146725	2.86%	0.365%
29	15.198	2226	2229	2250	rVB4	248325	732200	14.28%	1.823%
30	15.445	2268	2271	2277	rVB	56564	71442	1.39%	0.178%
31	15.510	2277	2282	2287	rBV	1129836	1406609	27.43%	3.502%
32	15.757	2319	2324	2332	rVB	120962	176115	3.43%	0.438%
33	15.992	2359	2364	2370	rBV	106832	152606	2.98%	0.380%
34	16.804	2497	2502	2511	rVB3	83197	169693	3.31%	0.422%
35	18.174	2728	2735	2745	rVB6	133097	384769	7.50%	0.958%

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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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

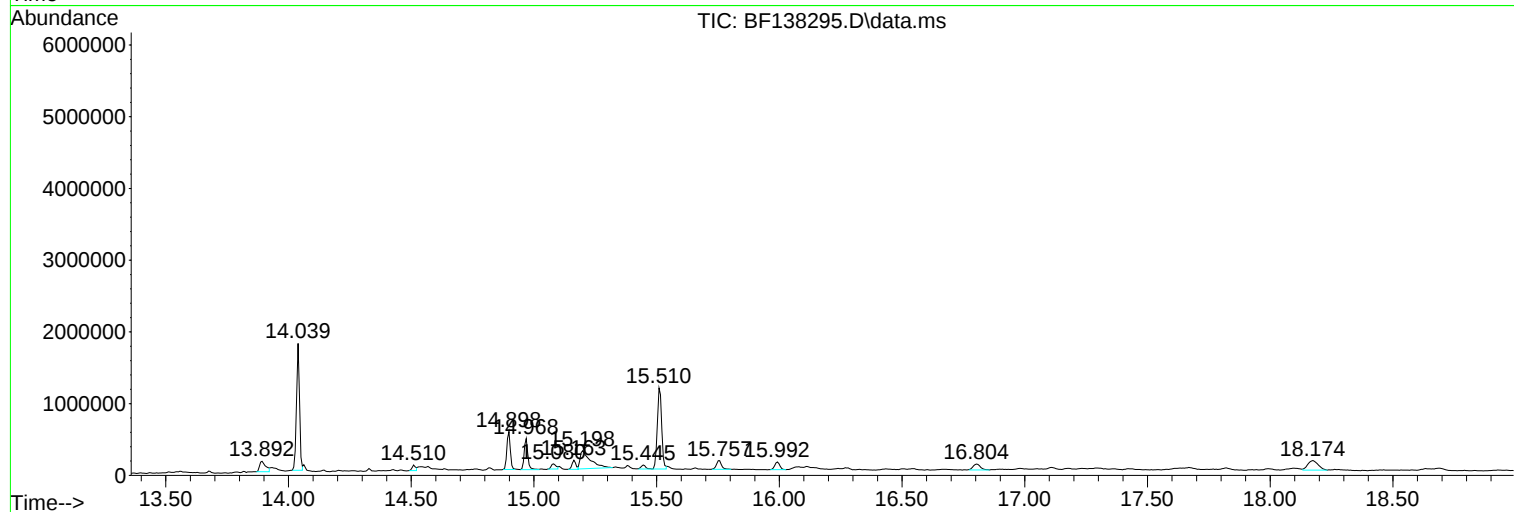
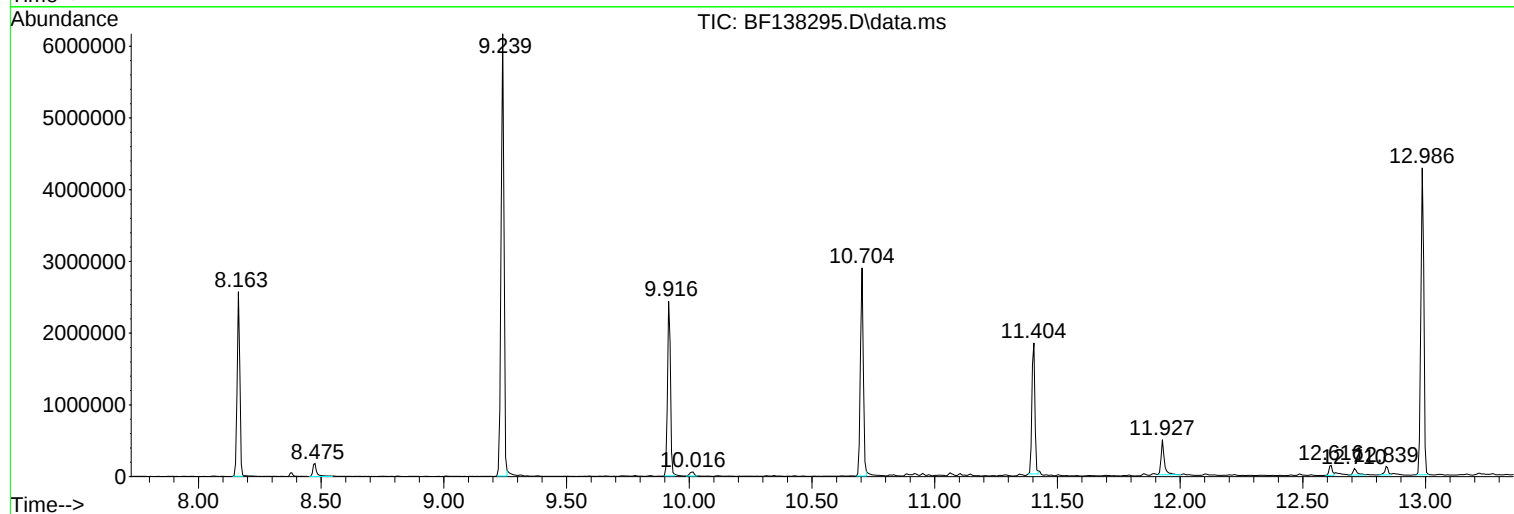
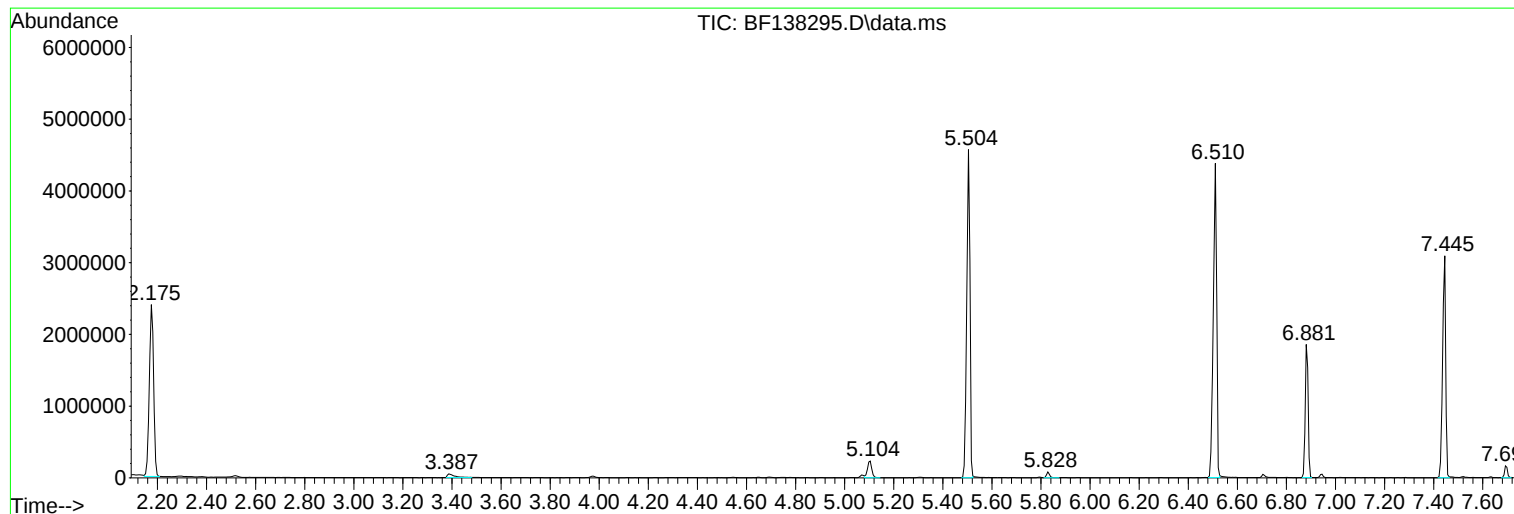
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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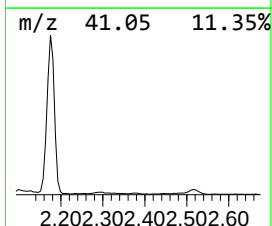
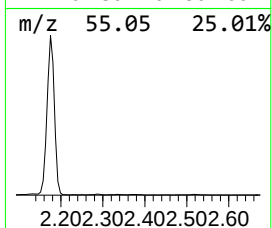
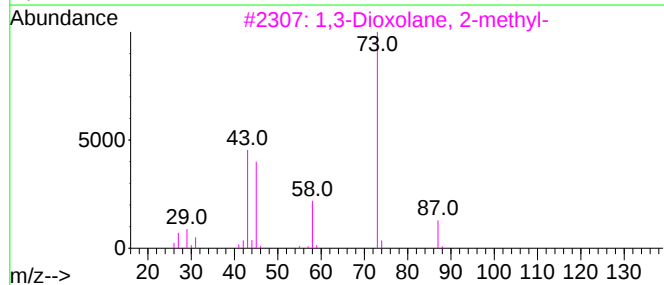
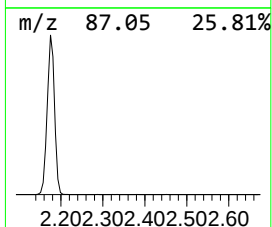
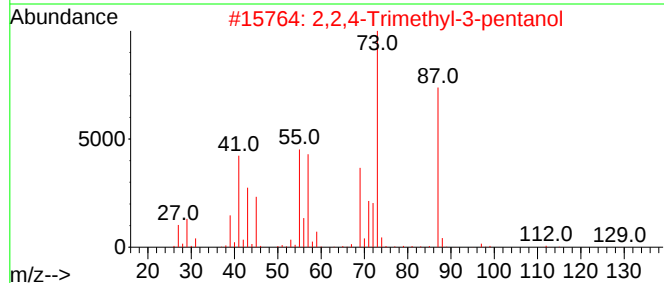
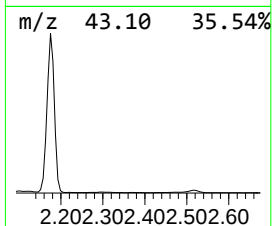
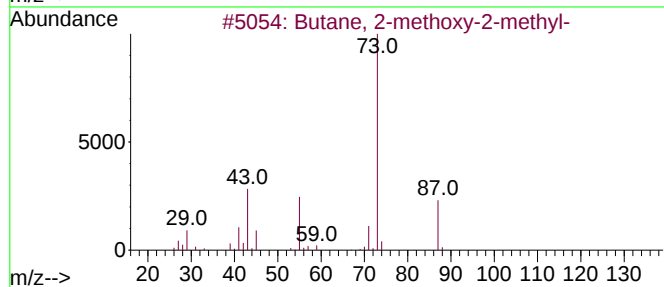
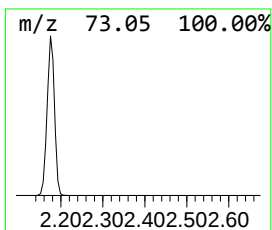
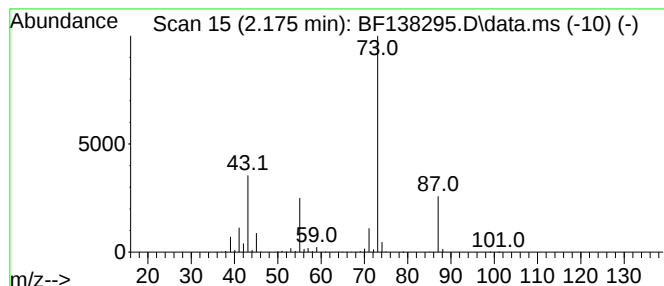
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	38.15 ng	2917910	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22



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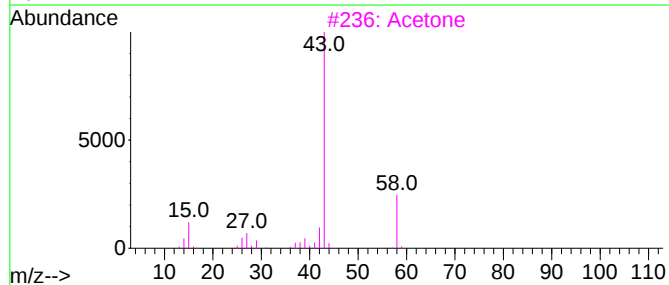
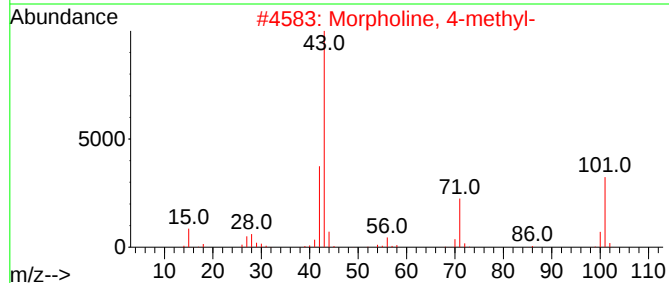
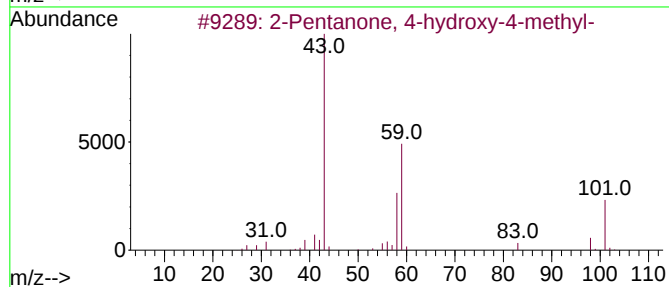
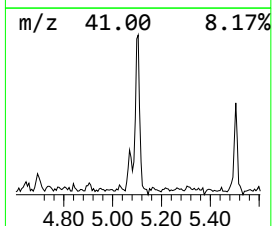
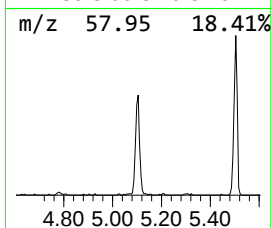
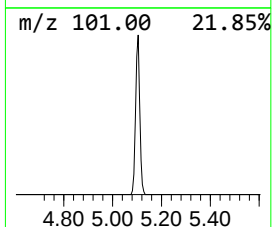
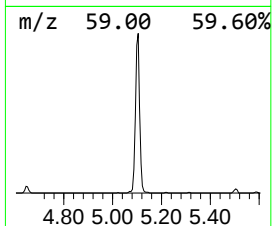
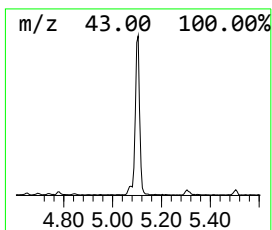
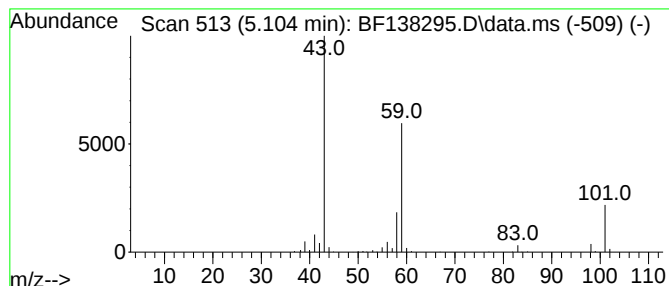
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	3.65 ng	279492	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
3	Acetone	58	C3H6O	000067-64-1	9		
4	Guanidine	59	CH5N3	000113-00-8	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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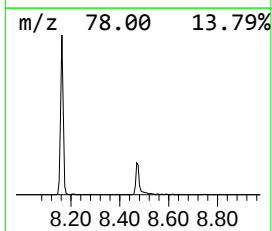
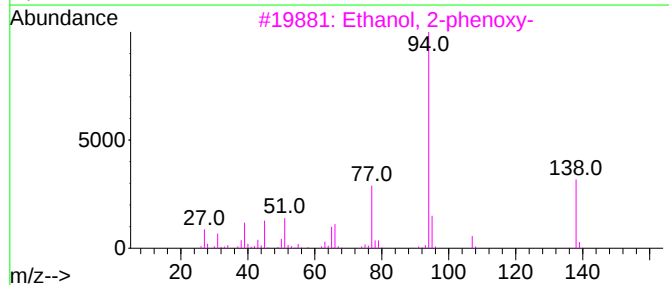
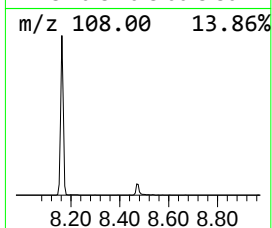
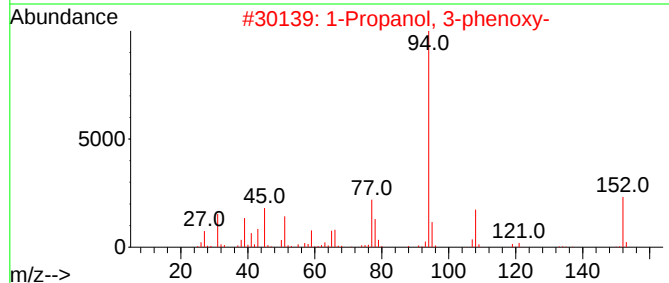
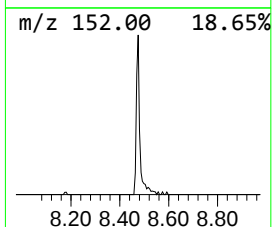
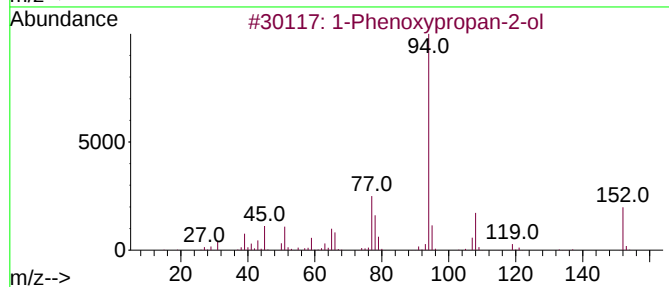
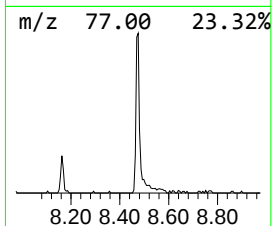
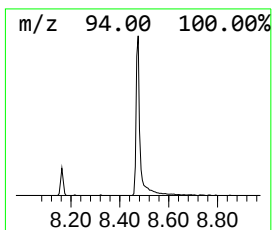
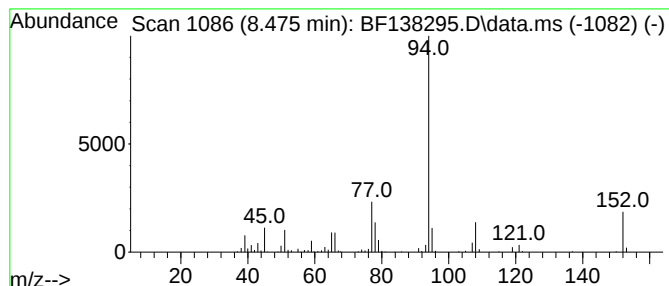
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.475	2.03 ng	200733	Naphthalene-d8	8.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59



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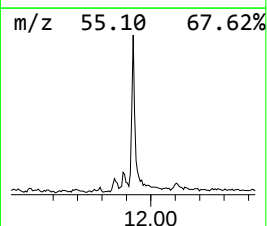
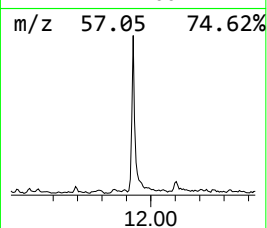
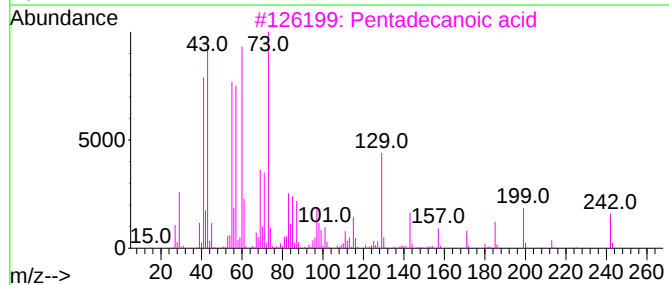
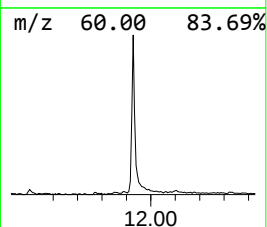
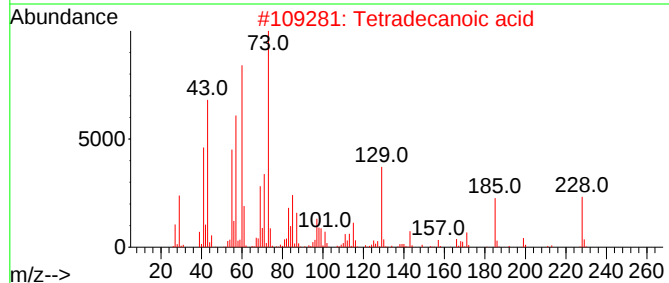
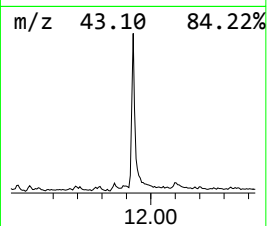
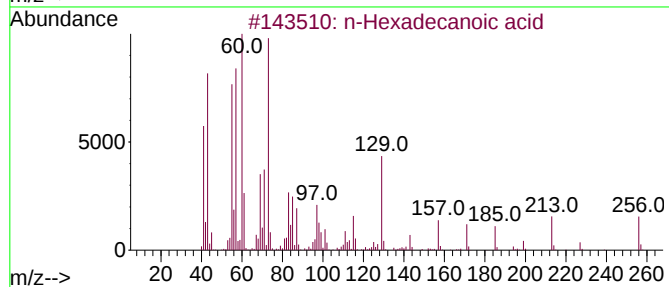
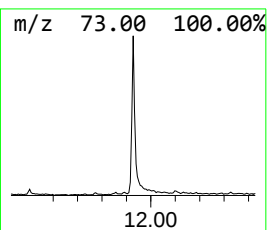
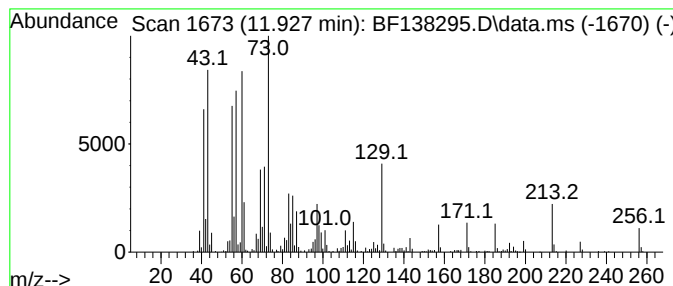
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	5.66 ng	442646	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	89
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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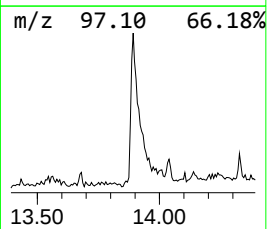
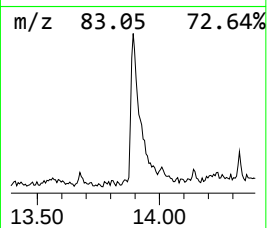
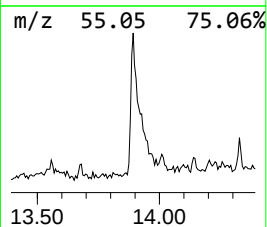
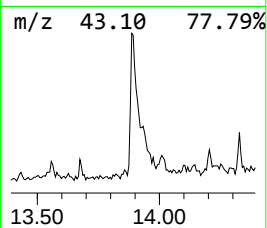
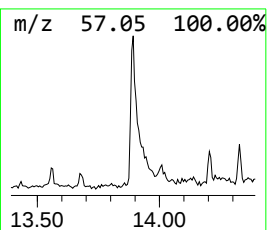
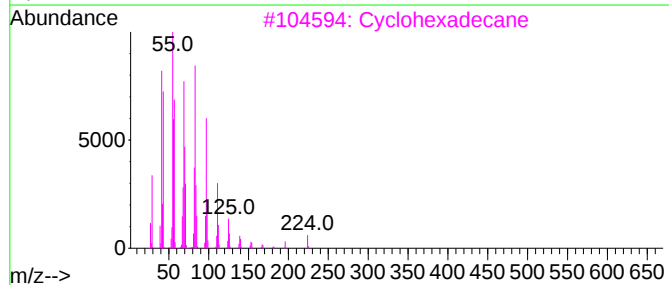
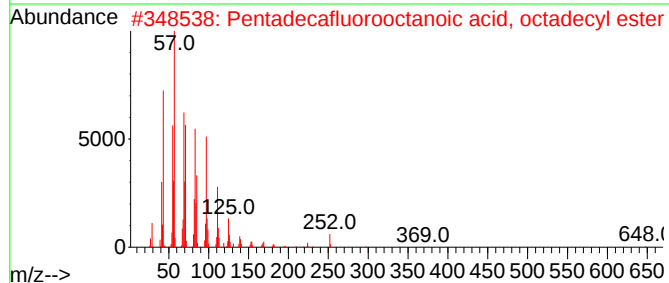
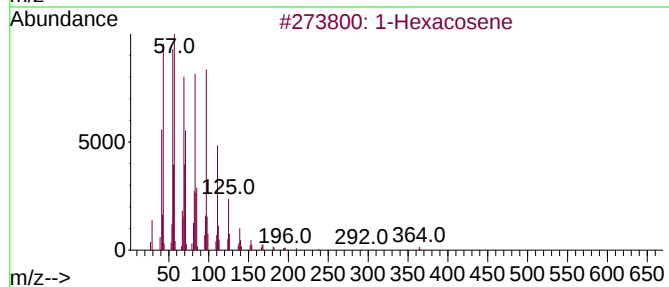
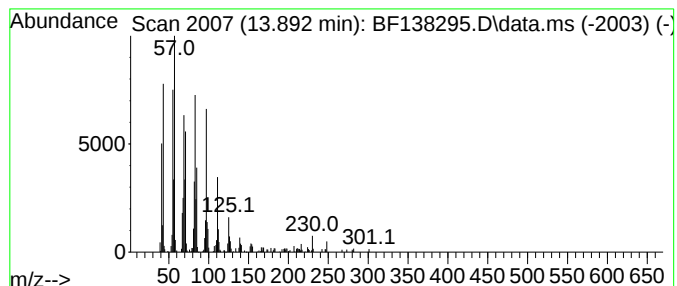
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Hexacosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	3.40 ng	260862	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosene	364	C26H52	018835-33-1	93
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
3			Cyclohexadecane	224	C16H32	000295-65-8	93
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			Behenic alcohol	326	C22H46O	000661-19-8	93



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Acq On : 21 Jun 2024 20:06
Operator : CG\JU
Sample : P2977-06
Misc :
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Instrument :
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ClientSampleId :
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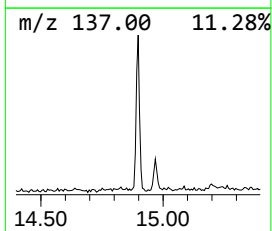
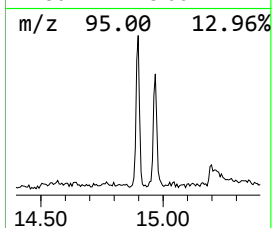
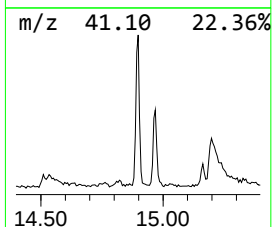
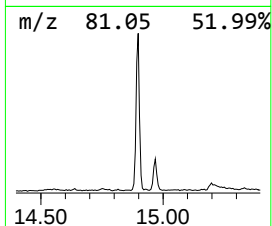
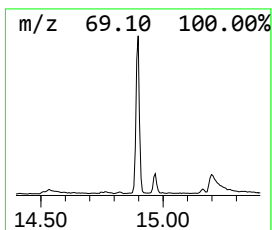
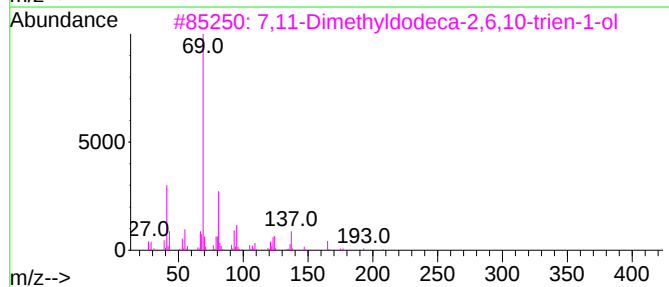
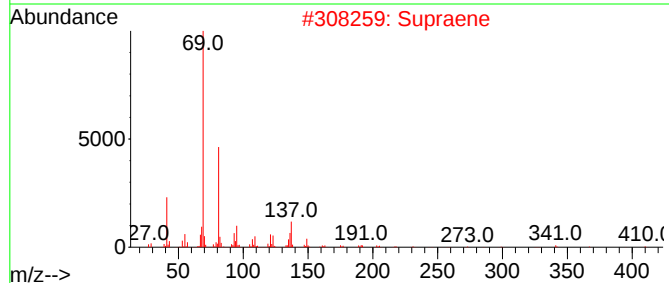
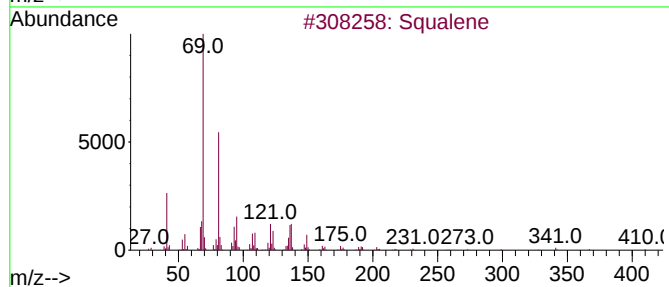
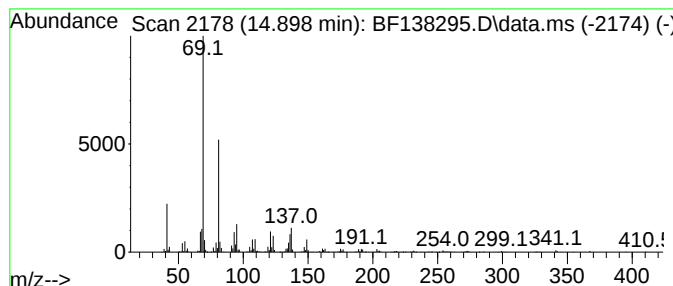
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	7.31 ng	514184	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	95
2			Supraene	410	C30H50	007683-64-9	91
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53



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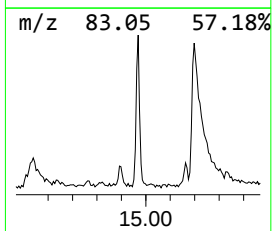
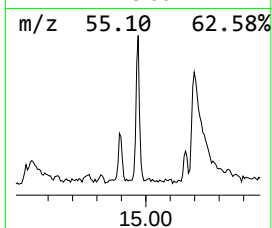
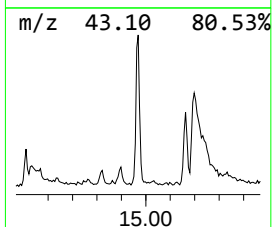
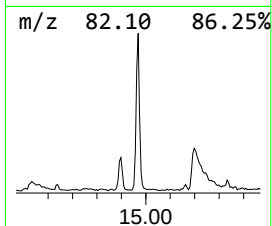
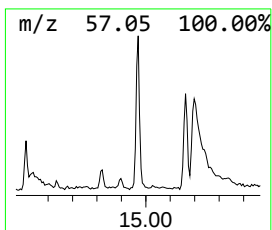
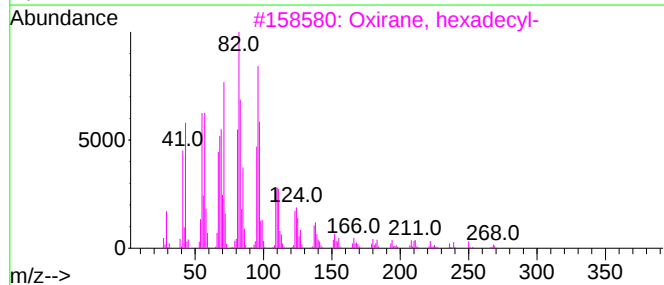
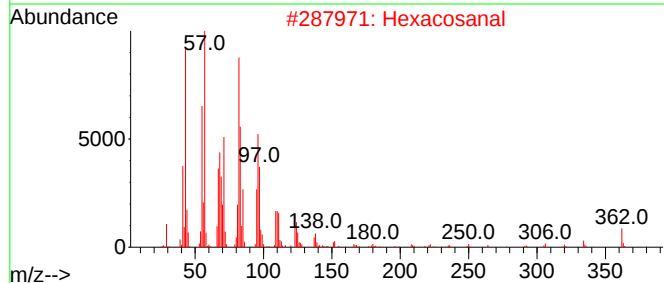
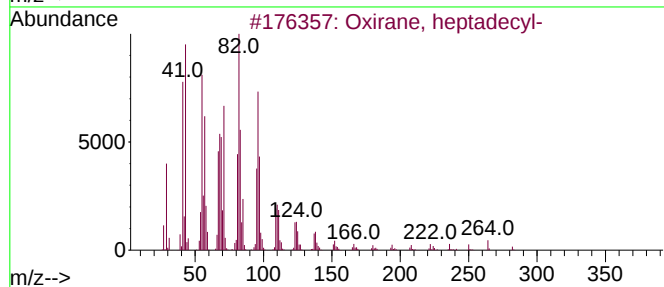
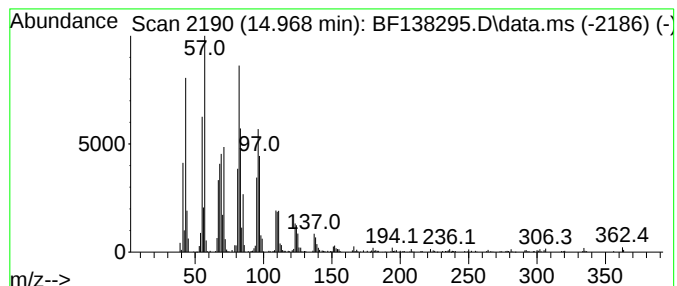
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Oxirane, heptadecyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	6.32 ng	444338	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95
2			Hexacosanal	380	C26H52O	026627-85-0	94
3			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4			Octadecanal	268	C18H36O	000638-66-4	91
5			17-Octadecenal	266	C18H34O	056554-86-0	91



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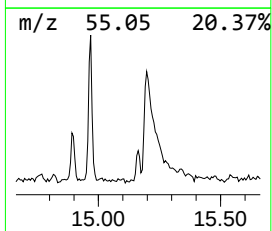
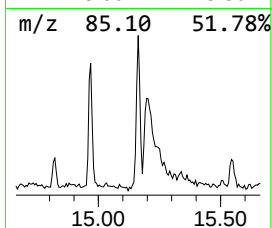
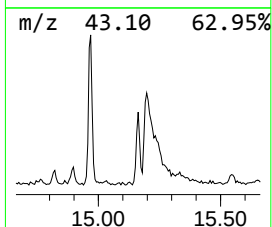
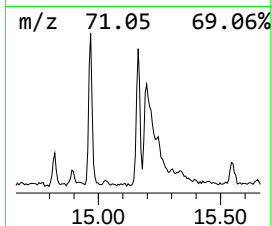
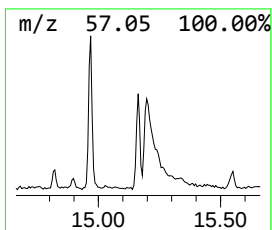
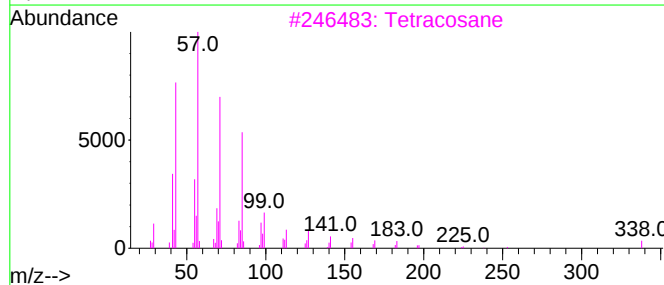
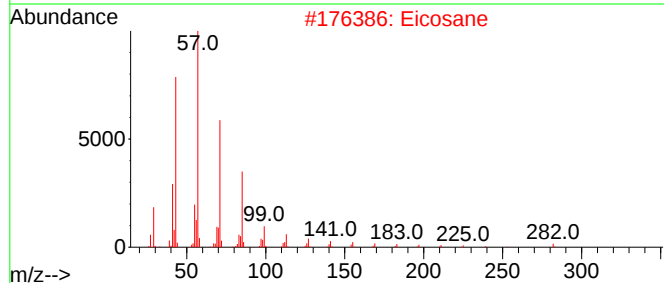
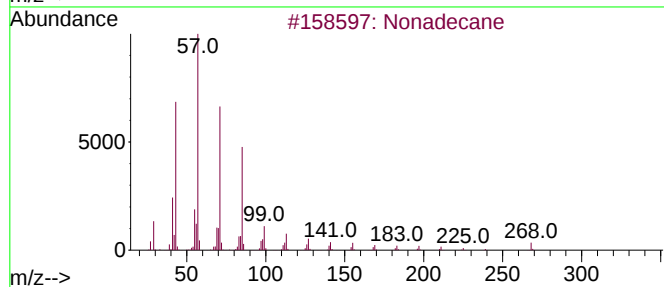
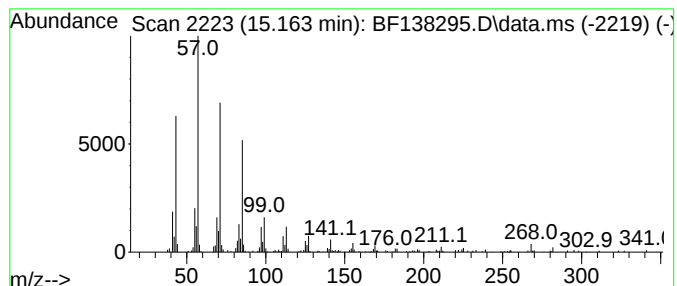
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Nonadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	2.09 ng	146725	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	95
2			Eicosane	282	C20H42	000112-95-8	92
3			Tetracosane	338	C24H50	000646-31-1	90
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5			Triacontane	422	C30H62	000638-68-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
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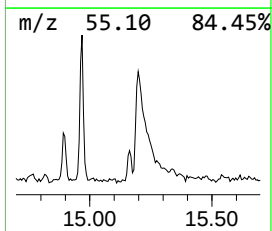
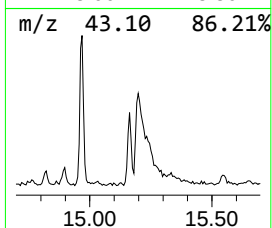
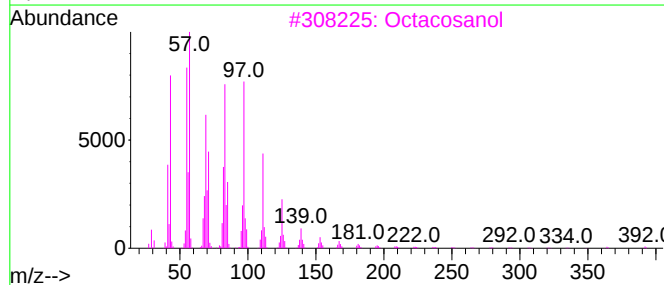
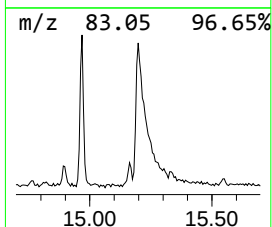
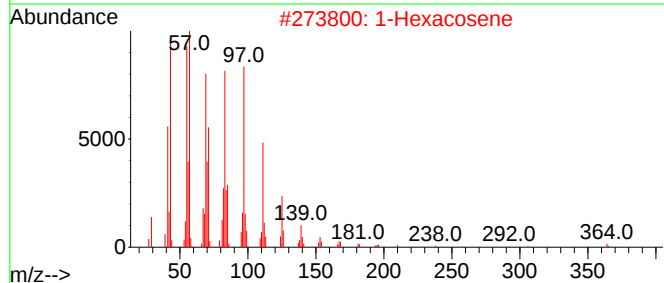
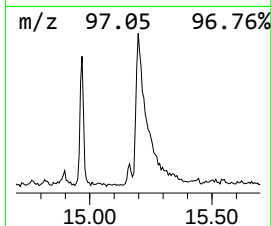
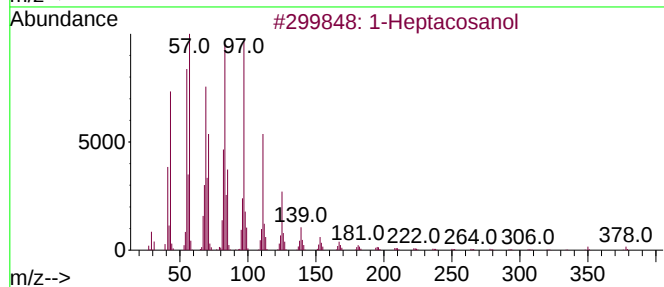
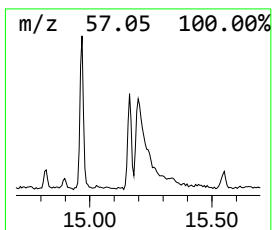
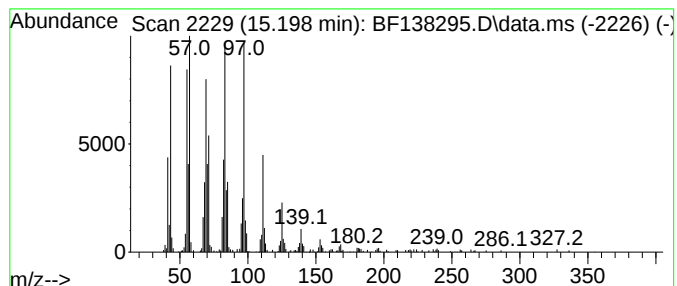
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1-Heptacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	10.41 ng	732200	Perylene-d12	15.510

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptacosanol	396	C27H56O	002004-39-9	95
2		1-Hexacosene	364	C26H52	018835-33-1	93
3		Octacosanol	410	C28H58O	000557-61-9	93
4		Behenic alcohol	326	C22H46O	000661-19-8	93
5		Octacosyl acetate	452	C30H60O2	018206-97-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
Data File : BF138295.D
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ALS Vial : 19 Sample Multiplier: 1

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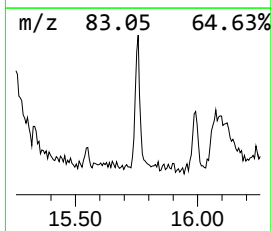
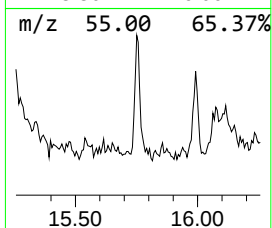
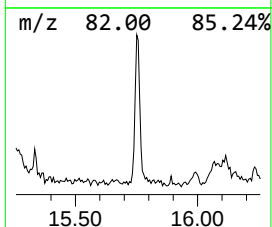
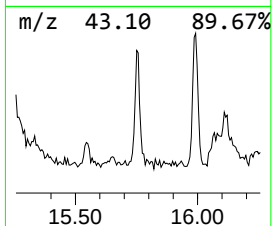
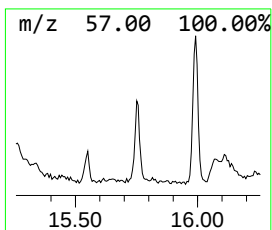
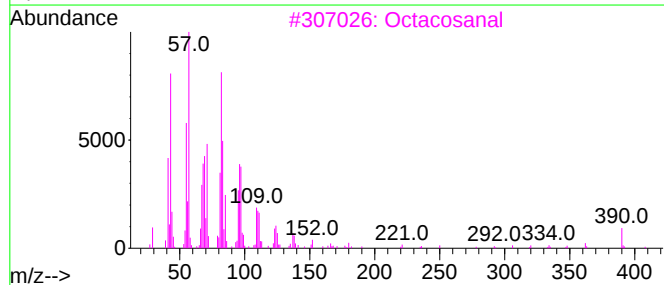
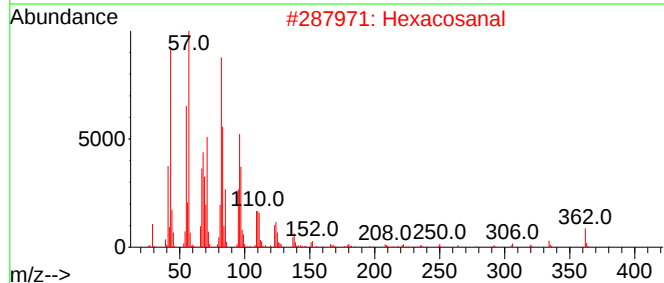
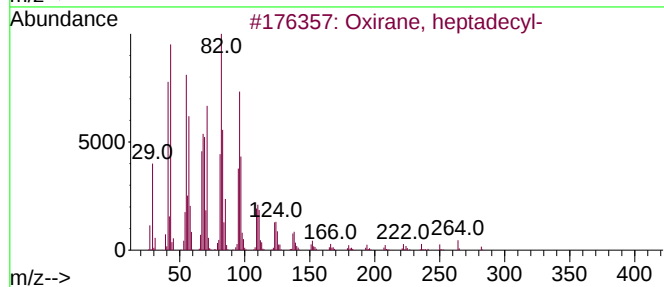
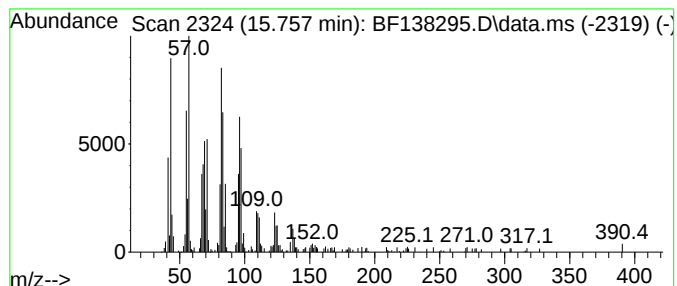
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Hexacosanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.757	2.50 ng	176115	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-		282	C19H38O	067860-04-2	95	
2	Hexacosanal		380	C26H52O	026627-85-0	94	
3	Octacosanal		408	C28H56O	022725-64-0	91	
4	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	91	
5	Octadecanal		268	C18H36O	000638-66-4	87	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
Data File : BF138295.D
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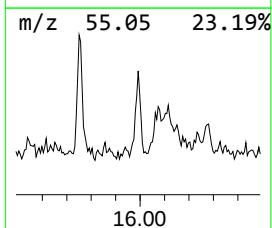
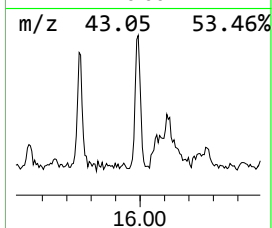
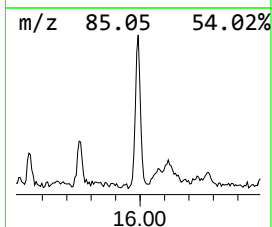
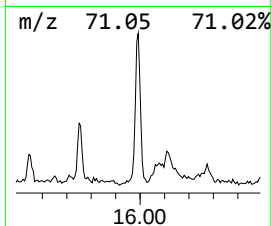
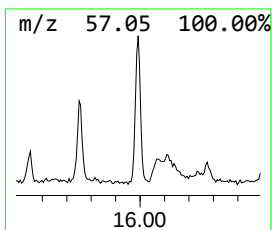
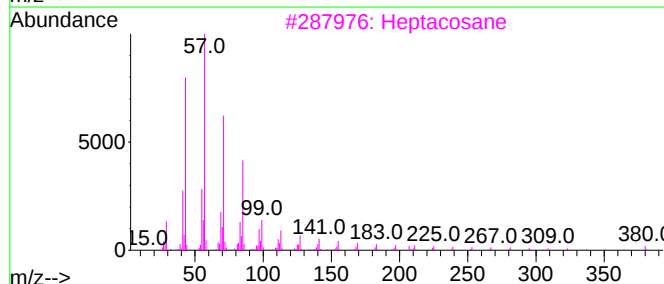
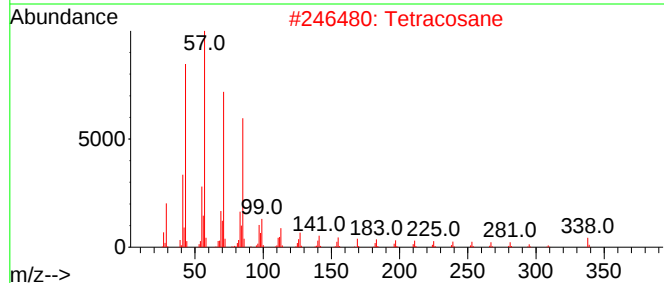
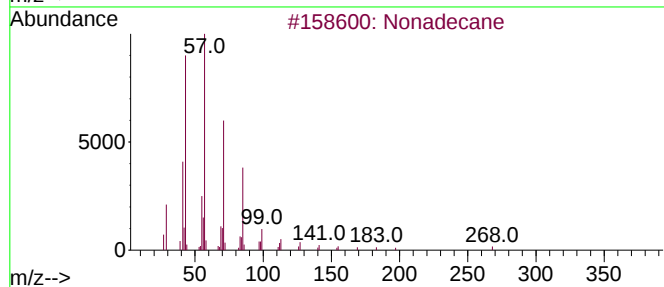
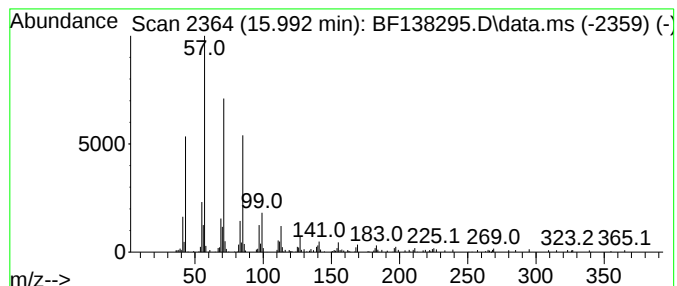
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Tetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.992	2.17 ng	152606	Perylene-d12	15.510

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	94
2		Tetracosane	338	C24H50	000646-31-1	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
5		Octacosane, 2-methyl-	408	C29H60	001560-98-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
Data File : BF138295.D
Acq On : 21 Jun 2024 20:06
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ALS Vial : 19 Sample Multiplier: 1

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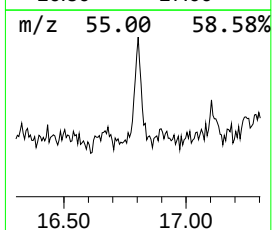
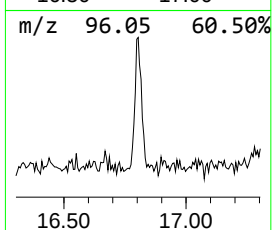
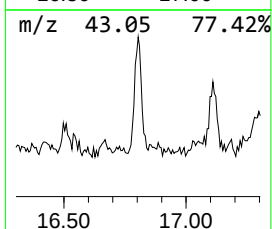
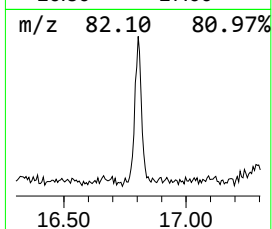
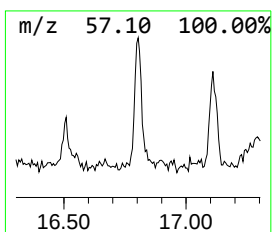
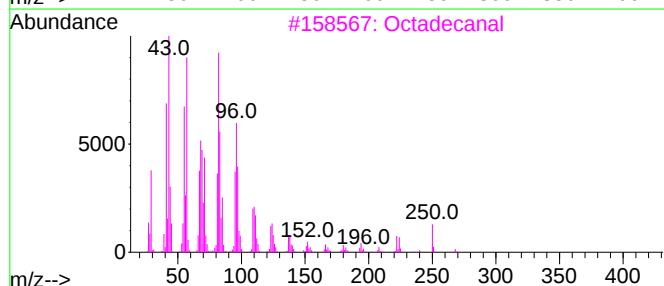
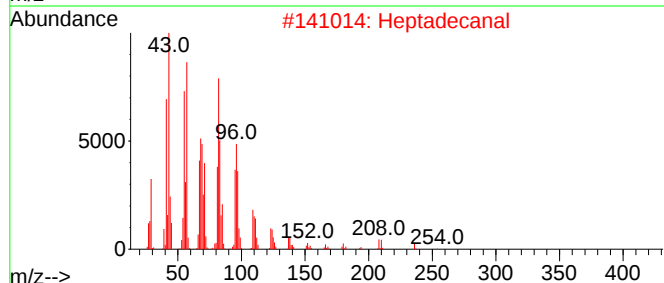
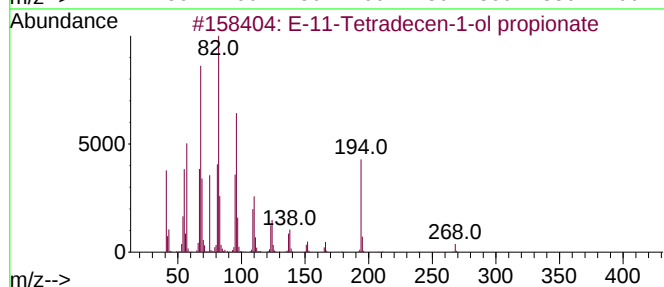
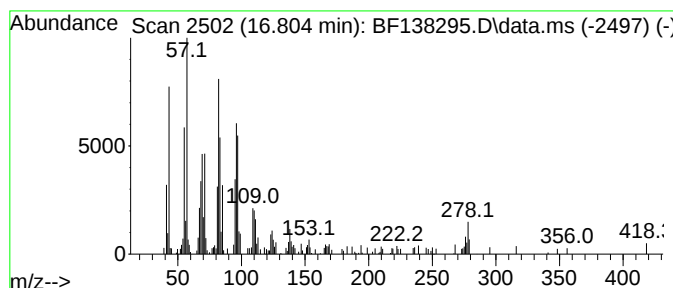
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 E-11-Tetradecen-1-ol propio... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.804	2.41 ng	169693	Perylene-d12	15.510

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-11-Tetradecen-1-ol propionate	268	C17H32O2	1000130-77-2	83	
2	Heptadecanal	254	C17H34O	1000376-70-0	80	
3	Octadecanal	268	C18H36O	000638-66-4	80	
4	Pentadecanal-	226	C15H30O	002765-11-9	80	
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	72	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
Data File : BF138295.D
Acq On : 21 Jun 2024 20:06
Operator : CG\JU
Sample : P2977-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-A6

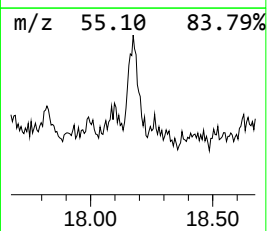
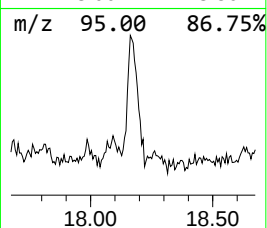
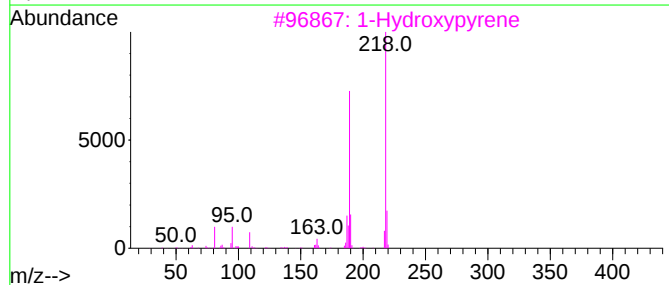
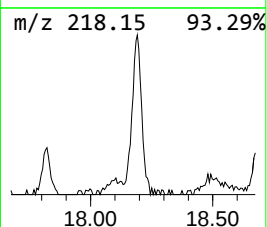
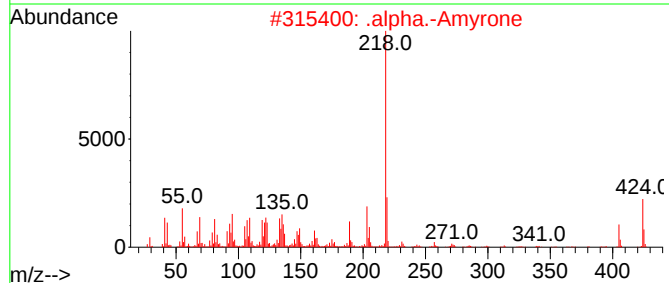
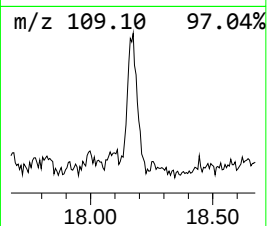
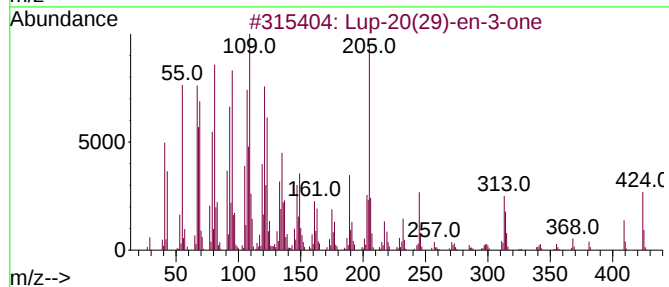
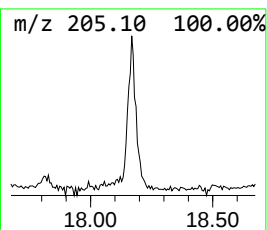
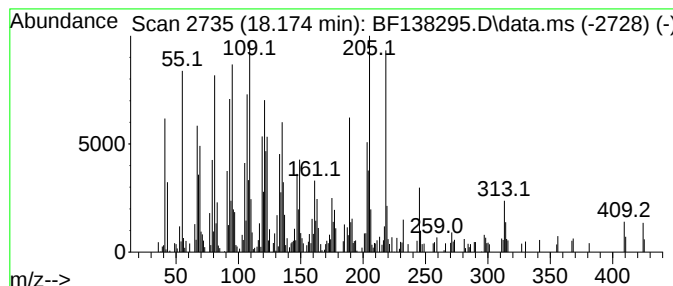
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Lup-20(29)-en-3-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.174	5.47 ng	384769	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	99
2			.alpha.-Amyrone	424	C30H48O	000638-96-0	95
3			1-Hydroxypyrene	218	C16H10O	005315-79-7	50
4			.beta.-Amyrone	424	C30H48O	000638-97-1	50
5			2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062124\
Data File : BF138295.D
Acq On : 21 Jun 2024 20:06
Operator : CG\JU
Sample : P2977-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OSTL-A6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.175	38.1	ng	2917910	1	6.881	1529590	20.0
2-Pentanone, 4-...	5.104	3.6	ng	279492	1	6.881	1529590	20.0
1-Phenoxypropan...	8.475	2.0	ng	200733	2	8.163	1974080	20.0
n-Hexadecanoic ...	11.928	5.7	ng	442646	4	11.404	1564630	20.0
1-Hexacosene	13.892	3.4	ng	260862	5	14.039	1536220	20.0
Squalene	14.898	7.3	ng	514184	6	15.510	1406610	20.0
Oxirane, heptad...	14.968	6.3	ng	444338	6	15.510	1406610	20.0
Nonadecane	15.163	2.1	ng	146725	6	15.510	1406610	20.0
1-Heptacosanol	15.198	10.4	ng	732200	6	15.510	1406610	20.0
Hexacosanal	15.757	2.5	ng	176115	6	15.510	1406610	20.0
Tetracosane	15.992	2.2	ng	152606	6	15.510	1406610	20.0
E-11-Tetradecen...	16.804	2.4	ng	169693	6	15.510	1406610	20.0
Lup-20(29)-en-3...	18.174	5.5	ng	384769	6	15.510	1406610	20.0