

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
 Data File : BM026629.D
 Acq On : 01 Jul 2020 10:03
 Operator : JU/CG
 Sample : L3153-34
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP2-I

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_M\METHODS\8270-BM060520.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	4.993	352	358	374	rBV	1696044	2315524	30.02%	5.946%
2	6.563	618	625	642	rBV2	1665679	2706224	35.09%	6.949%
3	7.357	753	760	771	rVB	329135	511393	6.63%	1.313%
4	7.669	806	813	824	rVB	1223011	1843649	23.91%	4.734%
5	8.504	948	955	974	rBV	1081350	1757880	22.79%	4.514%
6	10.110	1221	1228	1243	rBV	397014	673394	8.73%	1.729%
7	12.622	1648	1655	1667	rBV	2644312	3729277	48.35%	9.576%
8	13.492	1797	1803	1816	rBV	266324	388443	5.04%	0.997%
9	14.016	1883	1892	1900	rBV	581710	863868	11.20%	2.218%
10	15.522	2141	2148	2161	rBV	2921095	3930099	50.96%	10.092%
11	16.774	2354	2361	2371	rBV	709368	1017333	13.19%	2.612%
12	17.710	2515	2520	2527	rBV2	49705	79398	1.03%	0.204%
13	19.339	2792	2797	2802	rBV	340594	423502	5.49%	1.087%
14	19.433	2807	2813	2824	rBV	6290493	7712324	100.00%	19.804%
15	20.292	2955	2959	2963	rVB	250428	293357	3.80%	0.753%
16	20.562	3001	3005	3012	rBV	98408	123724	1.60%	0.318%
17	20.739	3031	3035	3046	rBV	351378	534569	6.93%	1.373%
18	20.986	3072	3077	3082	rBV	988079	1201029	15.57%	3.084%
19	21.615	3177	3184	3191	rBV2	363579	785614	10.19%	2.017%
20	22.027	3250	3254	3258	rBV	129925	163013	2.11%	0.419%
21	22.233	3285	3289	3295	rBV2	154665	196138	2.54%	0.504%
22	22.492	3328	3333	3337	rBV	1077358	1412130	18.31%	3.626%
23	22.533	3337	3340	3349	rVB	251073	429063	5.56%	1.102%
24	22.998	3416	3419	3425	rVB	190092	311948	4.04%	0.801%
25	23.068	3426	3431	3441	rVB	780103	1332982	17.28%	3.423%
26	23.280	3463	3467	3476	rVB	316030	489298	6.34%	1.256%
27	23.580	3513	3518	3525	rVB	929612	1557025	20.19%	3.998%
28	23.662	3527	3532	3543	rVB	198222	458699	5.95%	1.178%
29	24.639	3693	3698	3707	rVB3	206026	440255	5.71%	1.130%
30	25.015	3758	3762	3772	rVB2	148470	355372	4.61%	0.913%
31	25.803	3889	3896	3910	rVB4	280336	907436	11.77%	2.330%

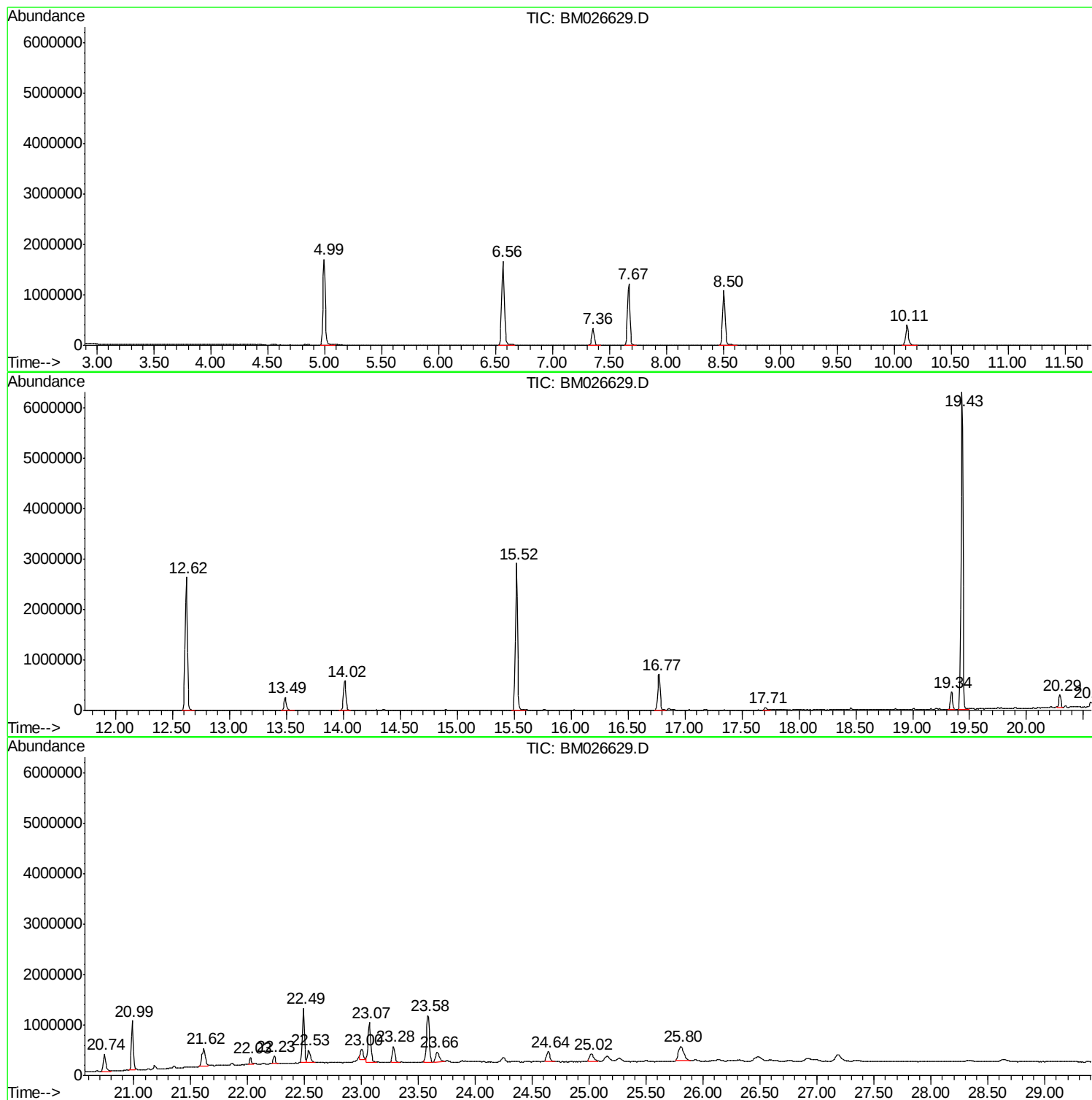
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM060520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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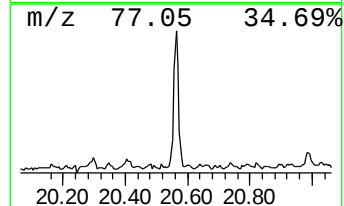
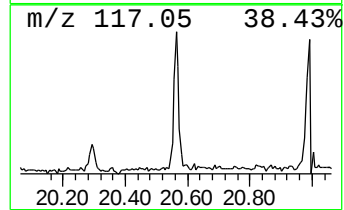
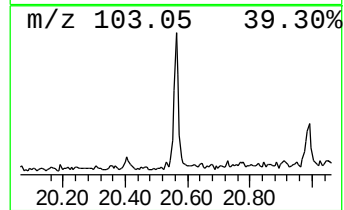
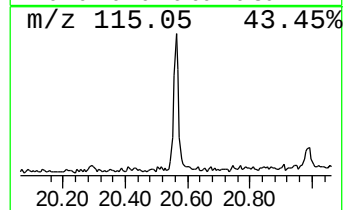
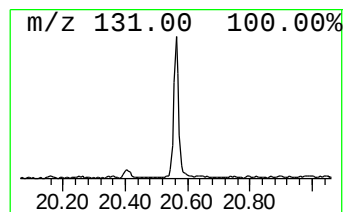
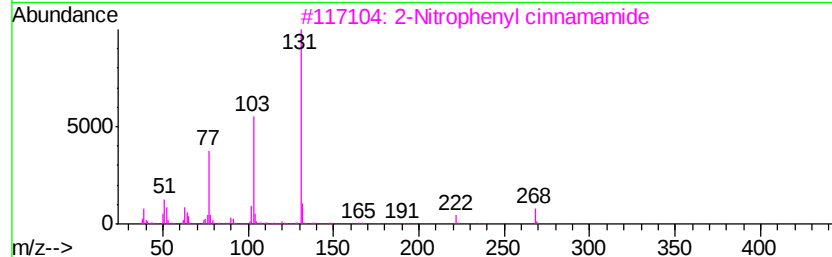
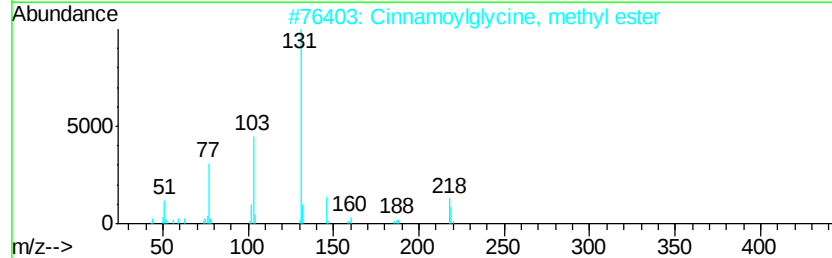
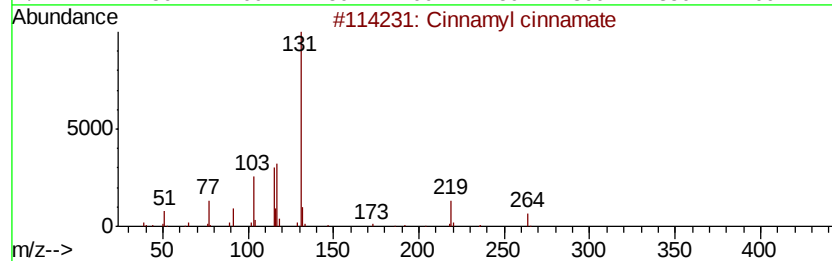
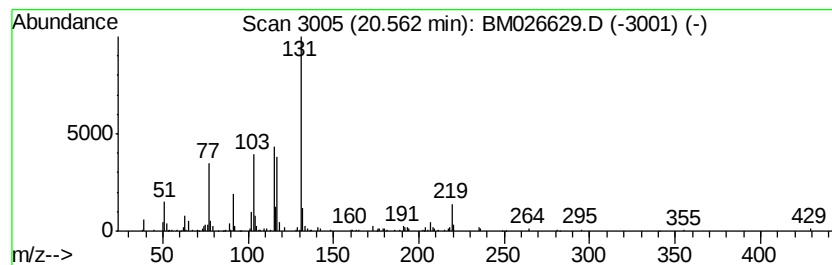
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM060520.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cinnamyl cinnamate Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.56	2.06 ng	123724	Chrysene-d12	20.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	80
2		Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	60
3		2-Nitrophenyl cinnamamide	268	C15H12N2O3	111273-37-1	43
4		trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	43
5		2-Propenoic acid, 3-phenyl-, 4-m...	238	C16H14O2	010519-07-0	43



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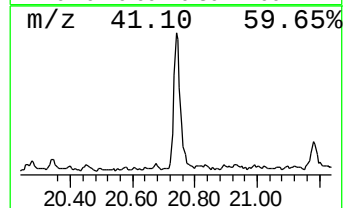
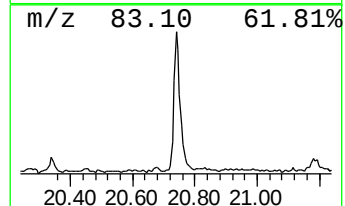
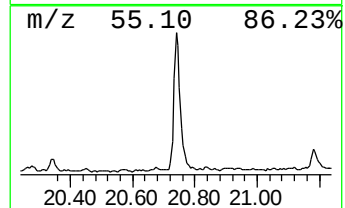
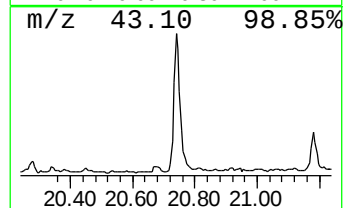
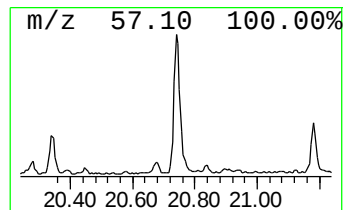
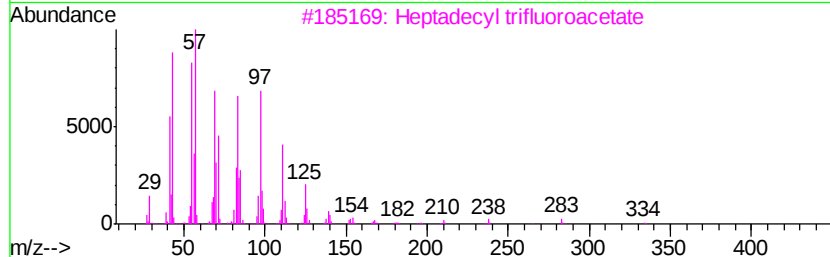
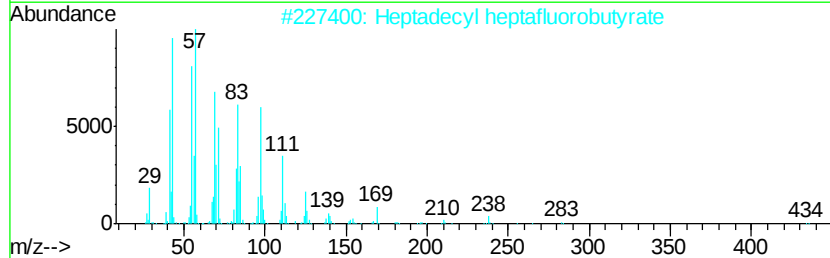
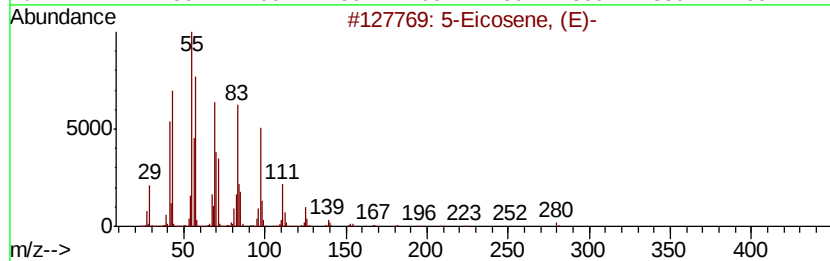
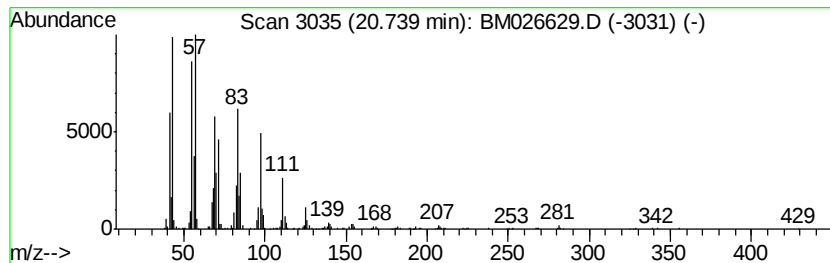
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Peak Number 5 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.74	8.90 ng	534569	Chrysene-d12	20.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Eicosene, (E)-	280	C20H40	074685-30-6	94
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



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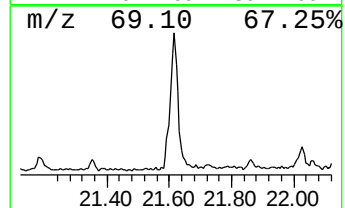
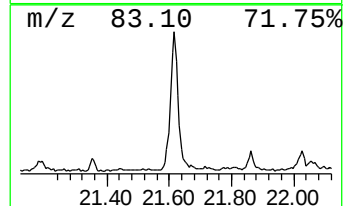
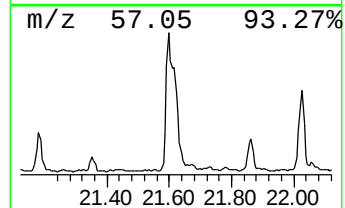
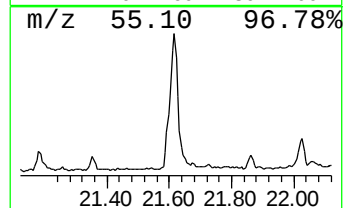
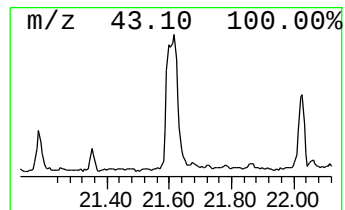
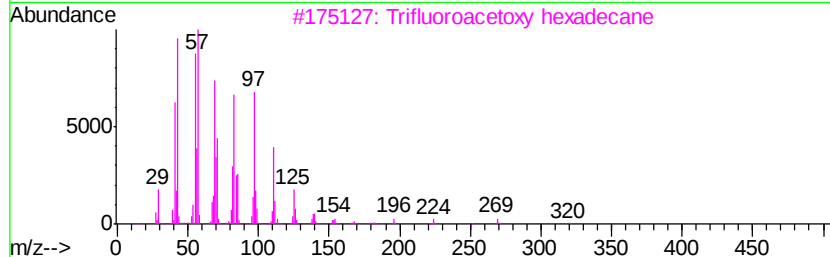
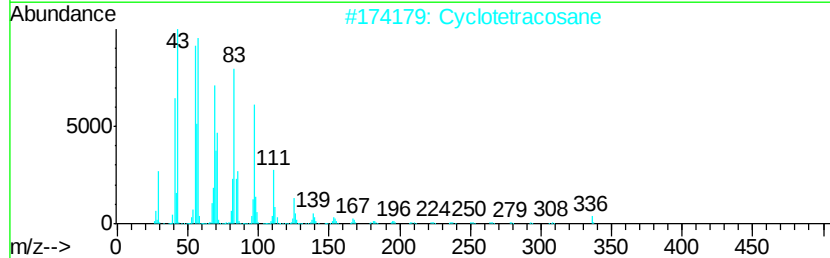
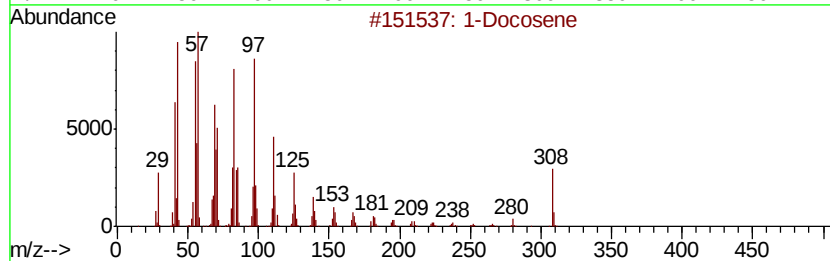
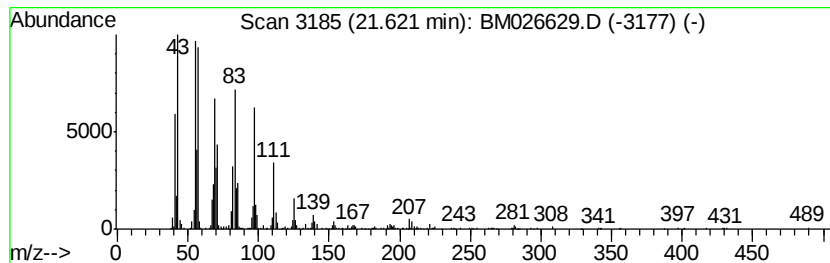
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Peak Number 6 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.62	13.08 ng	785614	Chrysene-d12	20.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	99
2	Cyclotetracosane		336	C24H48	000297-03-0	95
3	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	94
4	Octadecyl trifluoroacetate		366	C20H37F3O2	079392-43-1	94
5	Heptadecyl trifluoroacetate		352	C19H35F3O2	1000351-87-0	94



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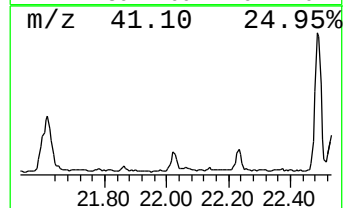
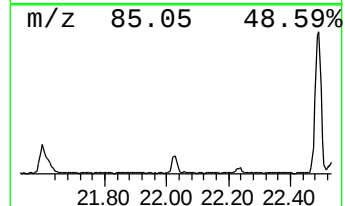
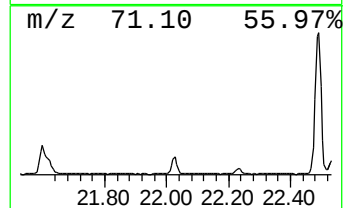
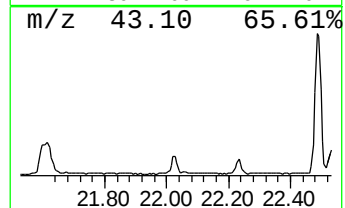
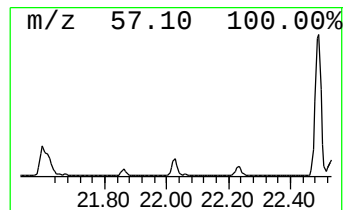
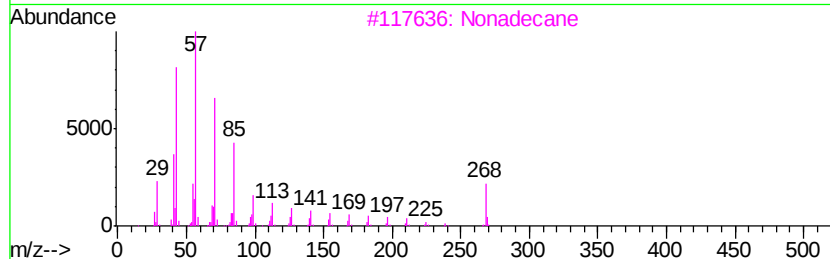
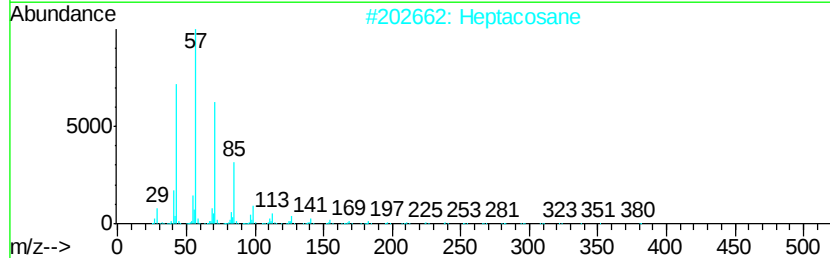
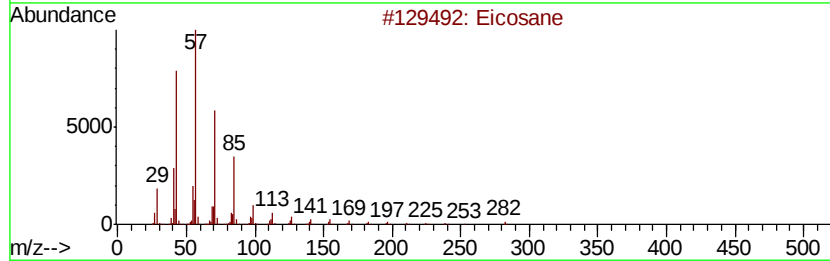
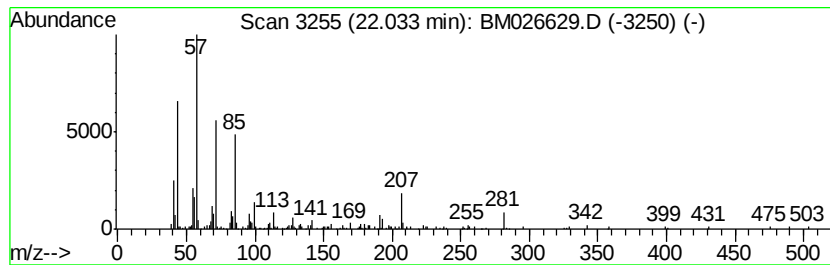
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Peak Number 7 Eicosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.03	2.45 ng	163013	Perylene-d12	23.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	98
2		Heptacosane	380	C27H56	000593-49-7	81
3		Nonadecane	268	C19H40	000629-92-5	81
4		Octadecane, 2-methyl-	268	C19H40	001560-88-9	74
5		Hexadecane	226	C16H34	000544-76-3	72



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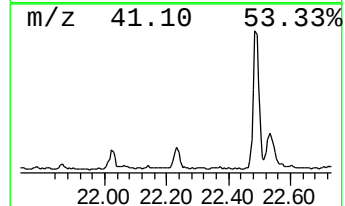
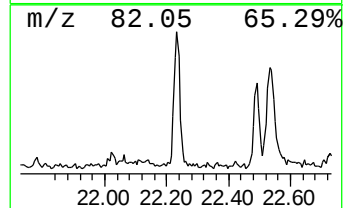
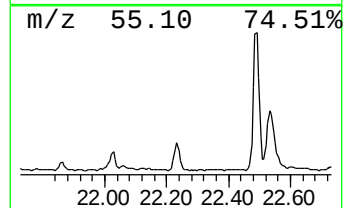
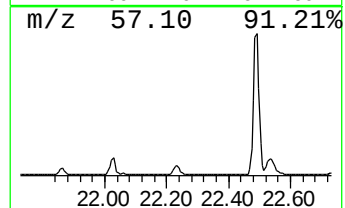
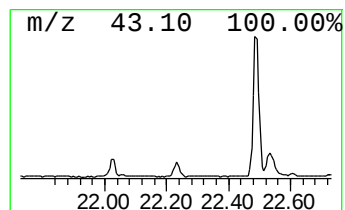
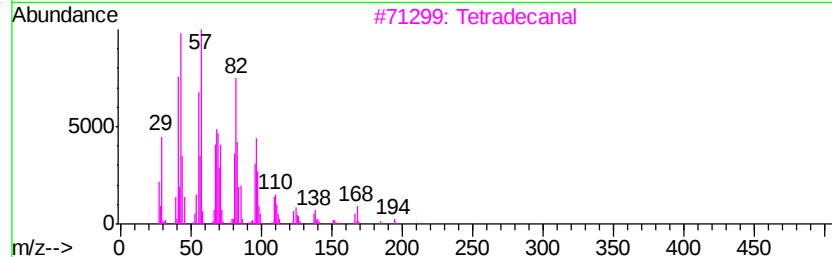
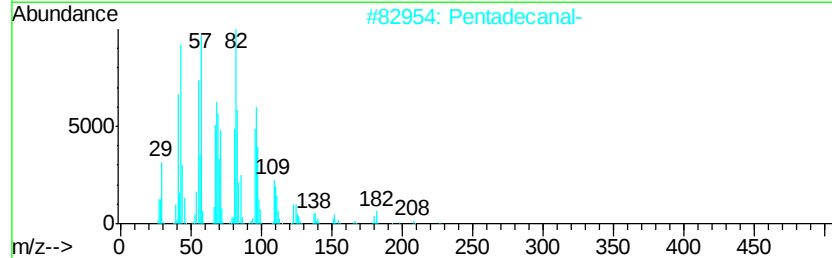
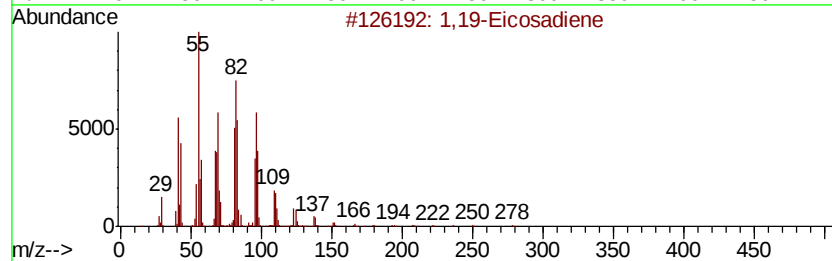
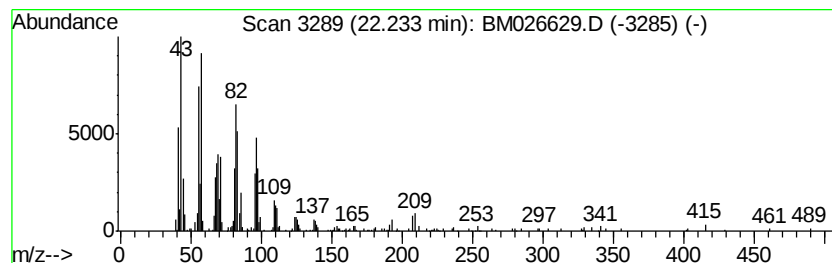
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Peak Number 8 1,19-Eicosadiene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.23	2.94 ng	196138	Perylene-d12	23.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,19-Eicosadiene	278	C20H38	014811-95-1	94
2		Pentadecanal-	226	C15H30O	002765-11-9	91
3		Tetradecanal	212	C14H28O	000124-25-4	91
4		Octadecanal	268	C18H36O	000638-66-4	87
5		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	81



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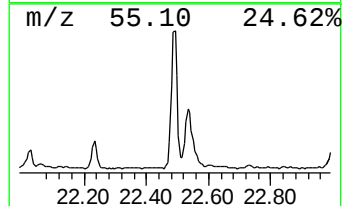
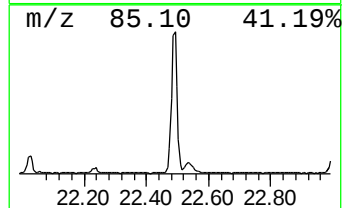
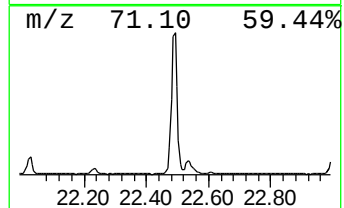
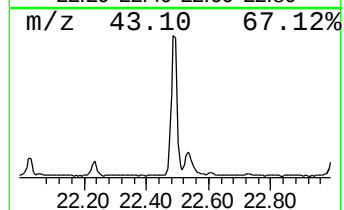
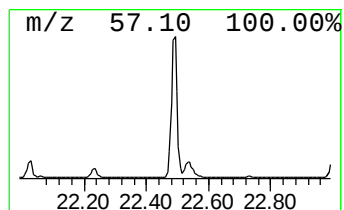
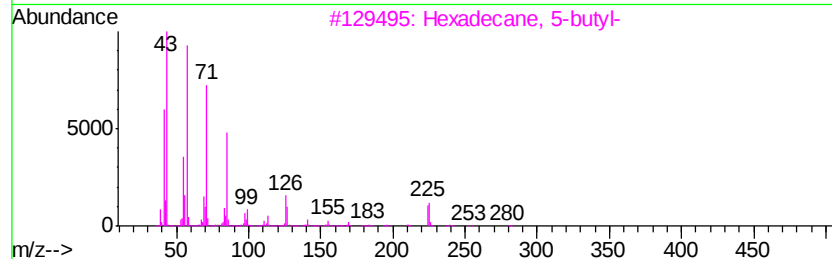
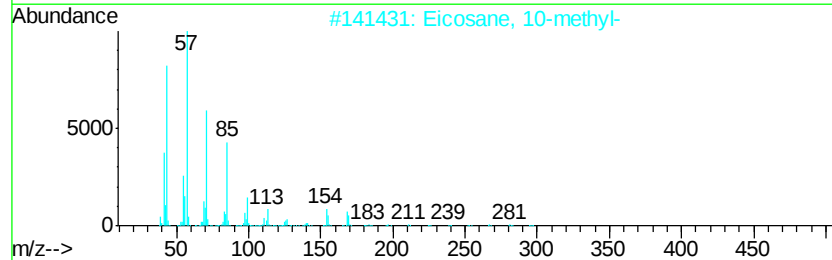
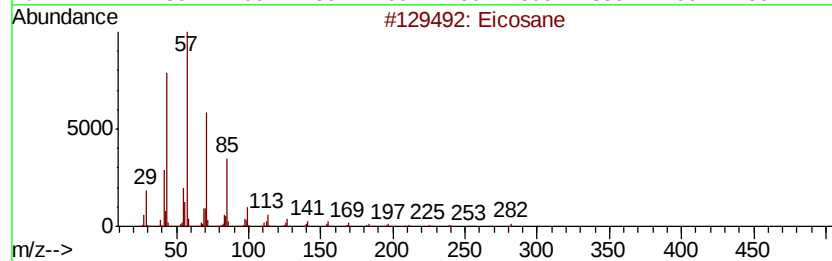
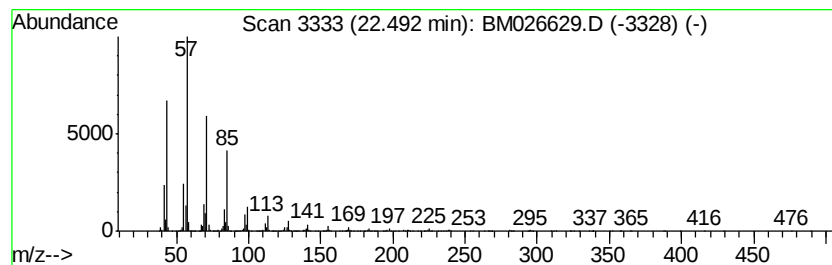
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane, 10-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.49	21.19 ng	1412130	Perylene-d12	23.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	97
2	Eicosane, 10-methyl-		296	C21H44	054833-23-7	93
3	Hexadecane, 5-butyl-		282	C20H42	006912-07-8	93
4	Pentadecane, 8-hexyl-		296	C21H44	013475-75-7	93
5	Heneicosane		296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
Data File : BM026629.D
Acq On : 01 Jul 2020 10:03
Operator : JU/CG
Sample : L3153-34
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP2-I

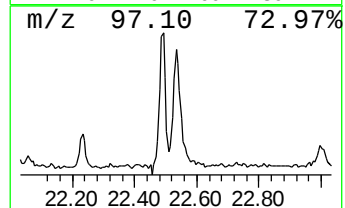
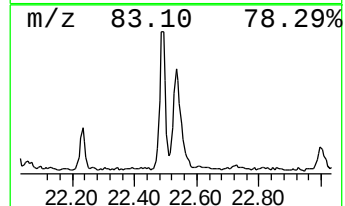
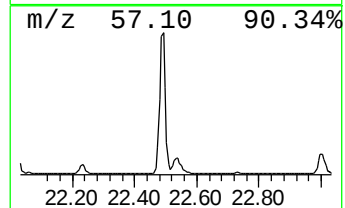
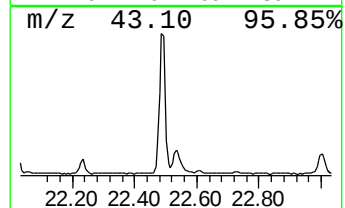
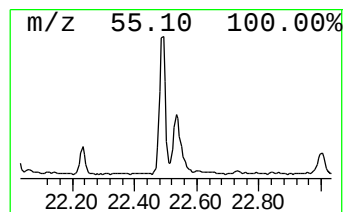
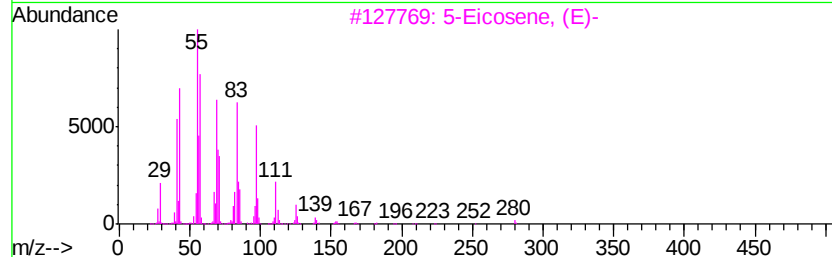
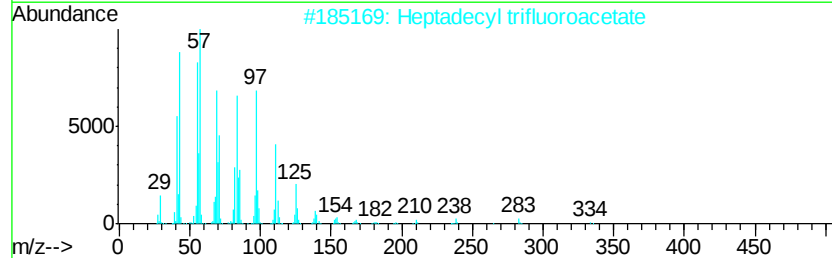
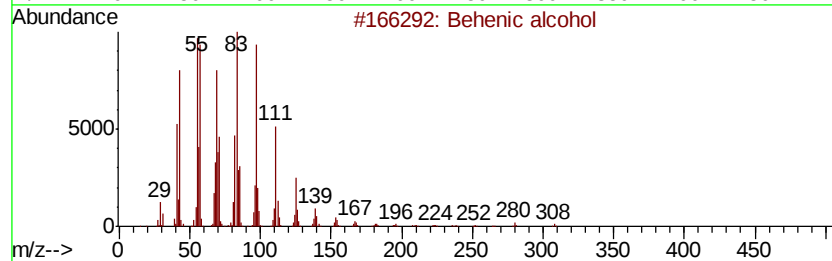
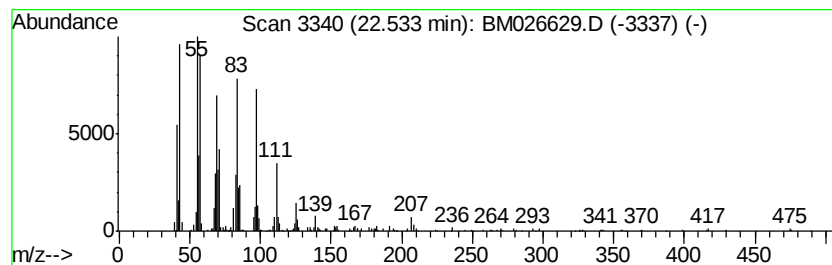
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Behenic alcohol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.53	6.44 ng	429063	Perylene-d12	23.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Behenic alcohol	326	C22H46O	000661-19-8	91
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	91
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	87
5		1-Heptacosanol	396	C27H56O	002004-39-9	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
Data File : BM026629.D
Acq On : 01 Jul 2020 10:03
Operator : JU/CG
Sample : L3153-34
Misc :
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ClientSampleId :
SP2-I

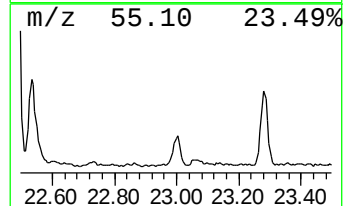
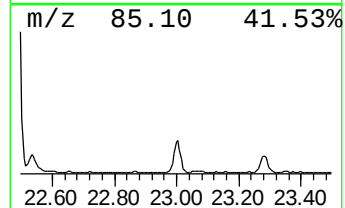
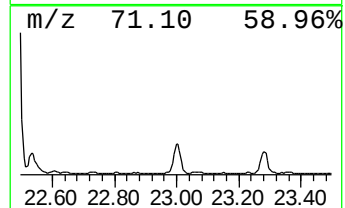
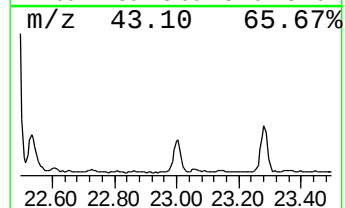
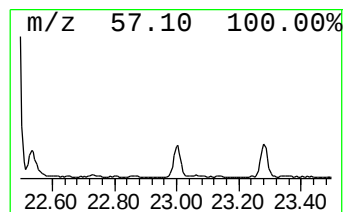
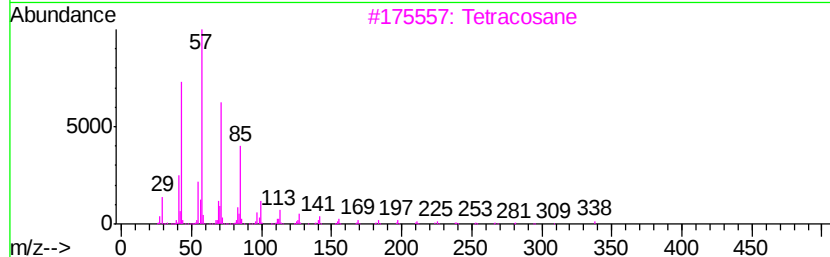
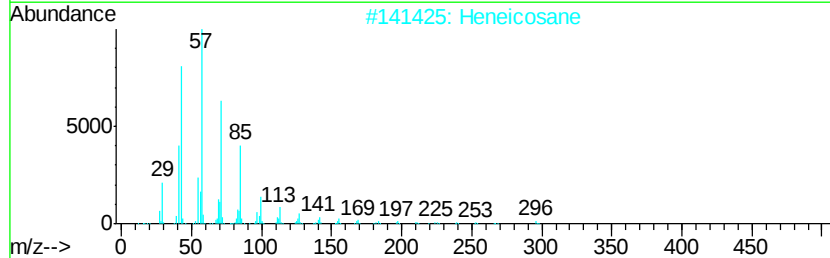
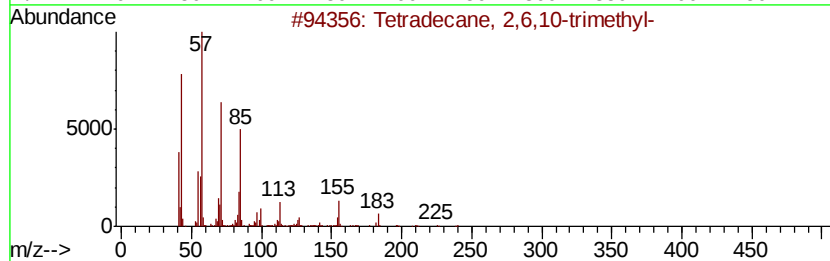
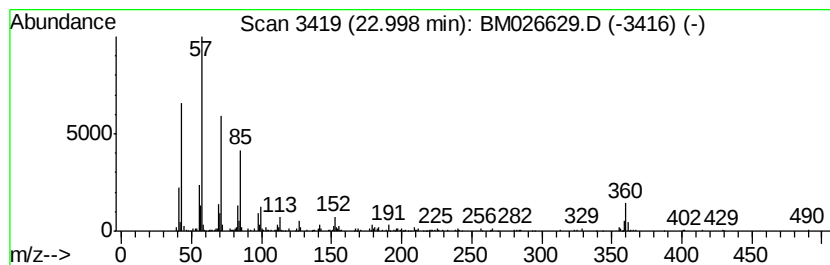
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetradecane, 2,6,10-trimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.00	4.68 ng	311948	Perylene-d12	23.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	81
2			Heneicosane	296	C21H44	000629-94-7	81
3			Tetracosane	338	C24H50	000646-31-1	81
4			Hexacosane	366	C26H54	000630-01-3	76
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
Data File : BM026629.D
Acq On : 01 Jul 2020 10:03
Operator : JU/CG
Sample : L3153-34
Misc :
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Instrument :
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ClientSampleId :
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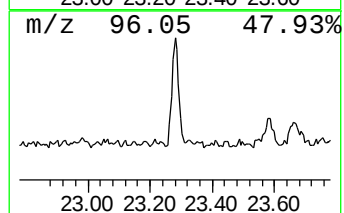
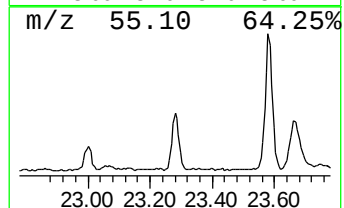
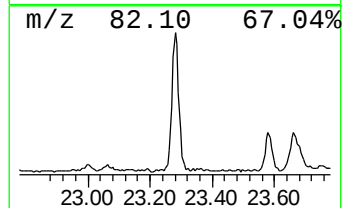
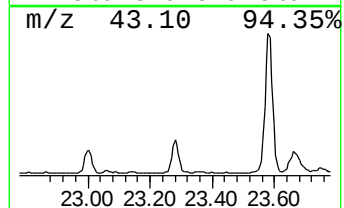
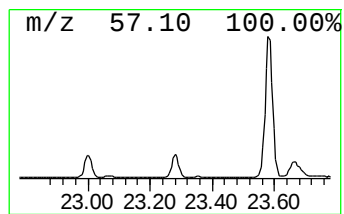
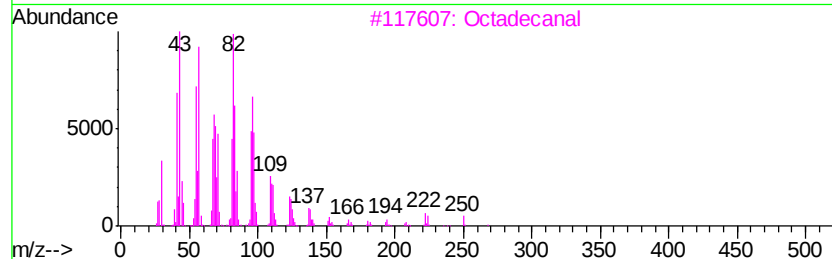
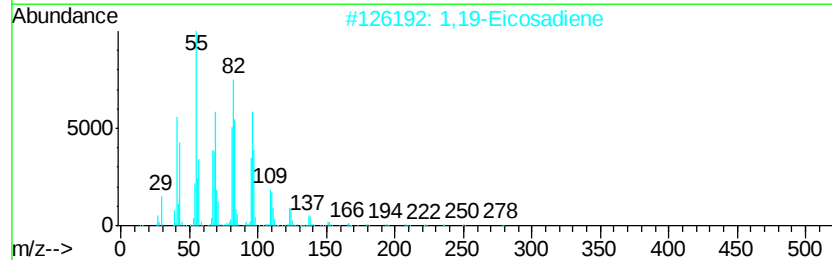
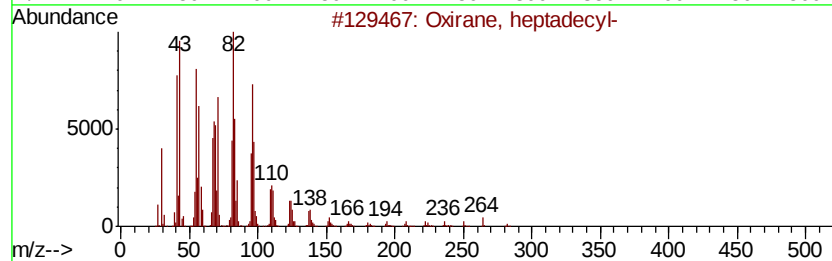
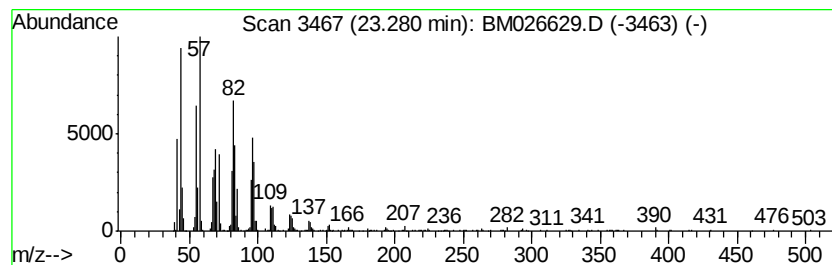
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Oxirane, heptadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.28	7.34 ng	489298	Perylene-d12	23.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	96
2		1,19-Eicosadiene	278	C20H38	014811-95-1	95
3		Octadecanal	268	C18H36O	000638-66-4	94
4		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
5		Pentadecanal-	226	C15H30O	002765-11-9	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
Data File : BM026629.D
Acq On : 01 Jul 2020 10:03
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Misc :
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ClientSampleId :
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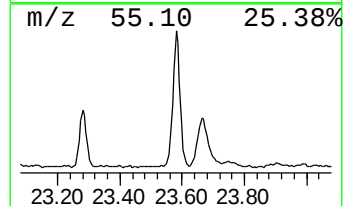
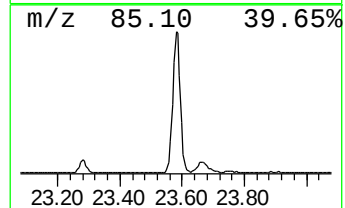
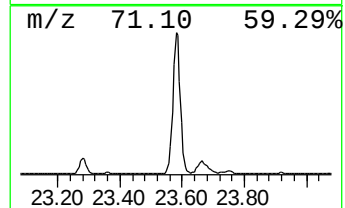
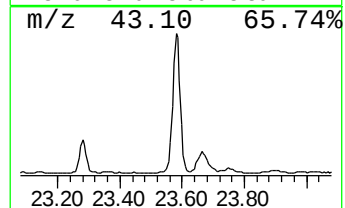
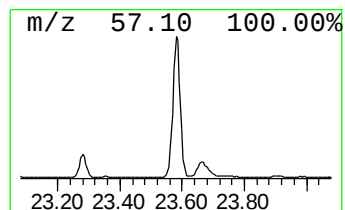
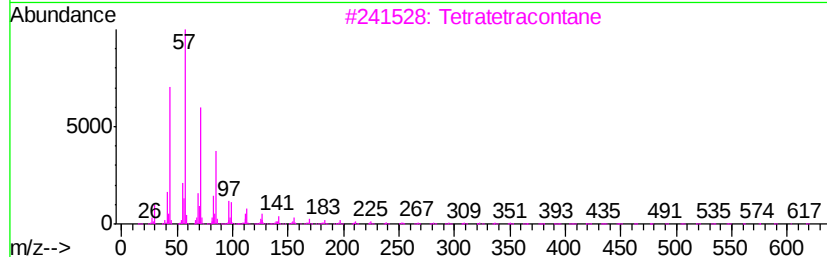
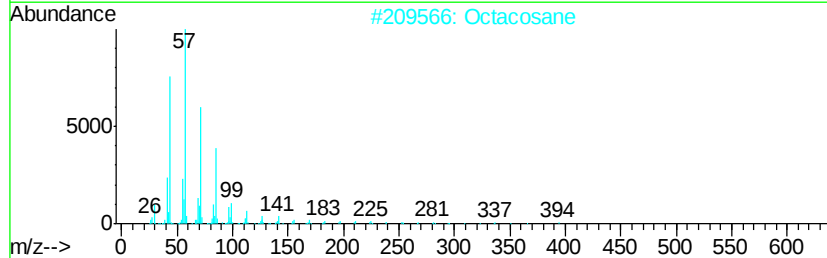
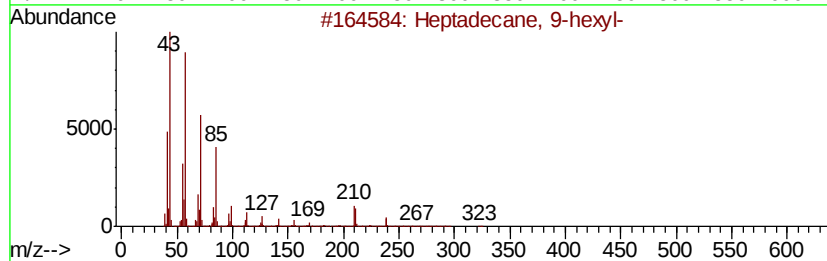
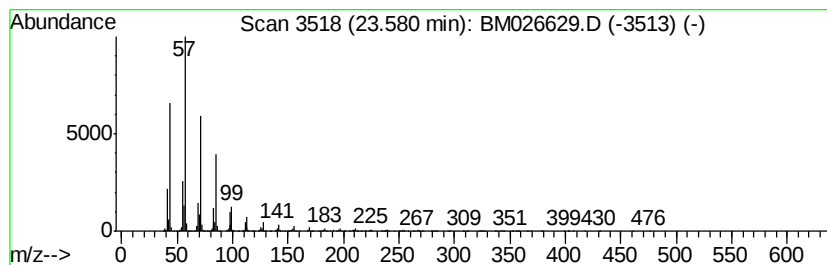
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Heptadecane, 9-hexyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.58	23.36 ng	1557030	Perylene-d12	23.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	94
2		Octacosane	394	C28H58	000630-02-4	91
3		Tetratetracontane	619	C44H90	007098-22-8	91
4		Heptacosane	380	C27H56	000593-49-7	91
5		Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
Data File : BM026629.D
Acq On : 01 Jul 2020 10:03
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Misc :
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ClientSampleId :
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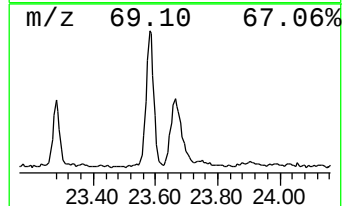
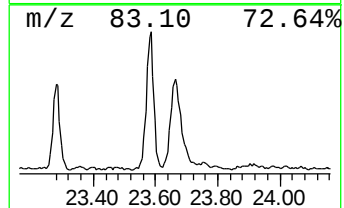
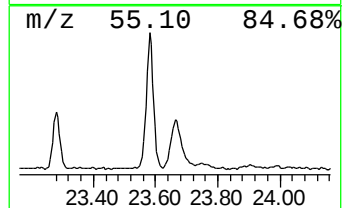
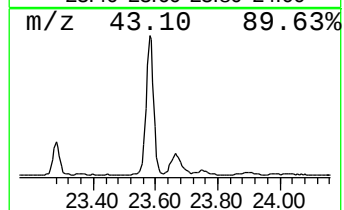
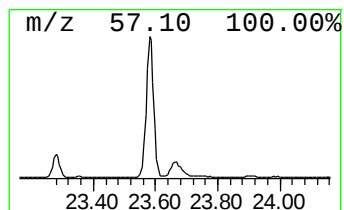
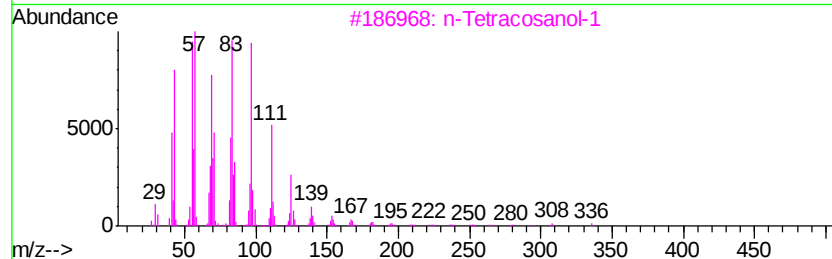
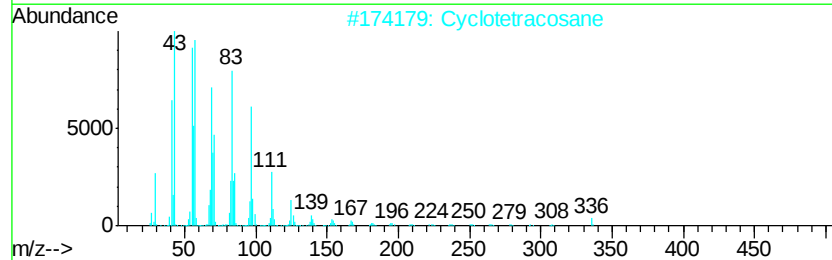
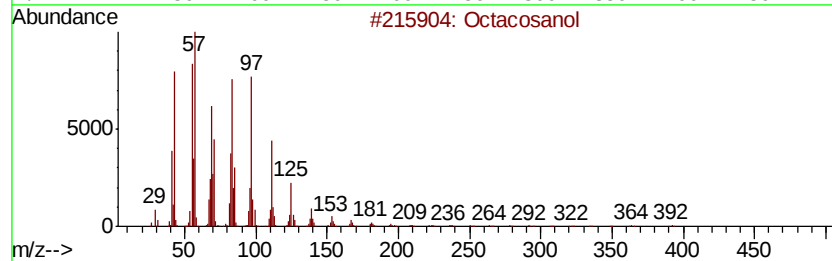
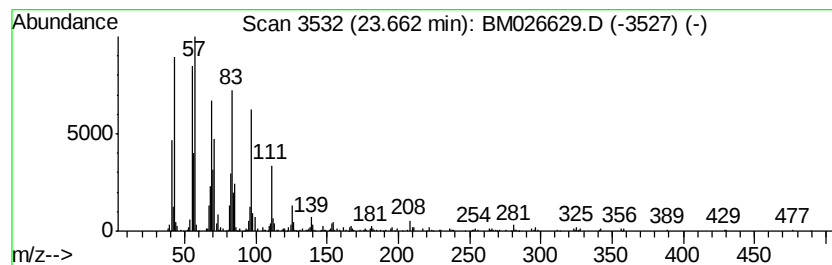
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Octacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.66	6.88 ng	458699	Perylene-d12	23.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanol	410	C28H58O	000557-61-9	91
2			Cyclotetracosane	336	C24H48	000297-03-0	90
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4			1-Heptacosanol	396	C27H56O	002004-39-9	87
5			1-Nonadecene	266	C19H38	018435-45-5	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
Data File : BM026629.D
Acq On : 01 Jul 2020 10:03
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ClientSampleId :
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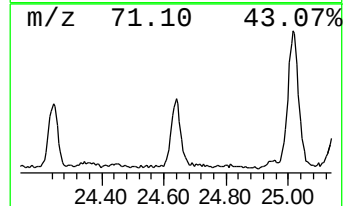
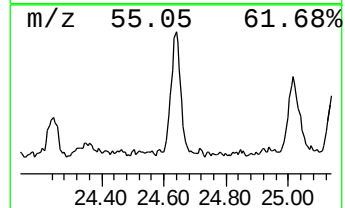
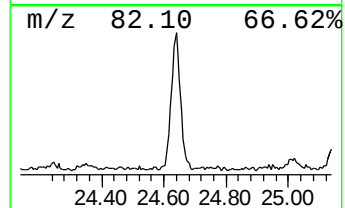
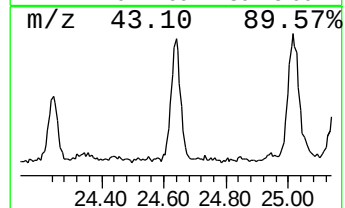
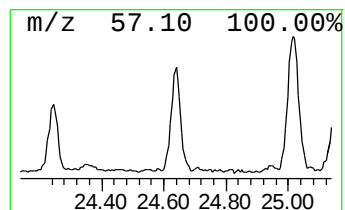
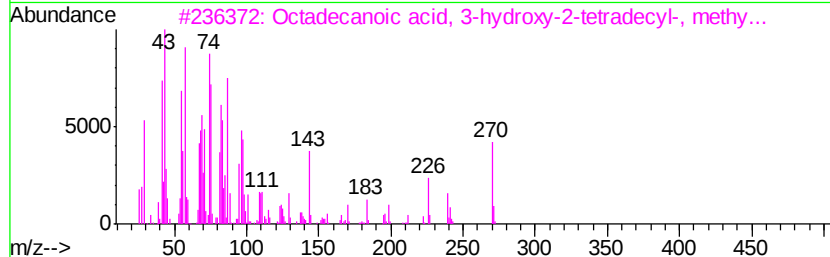
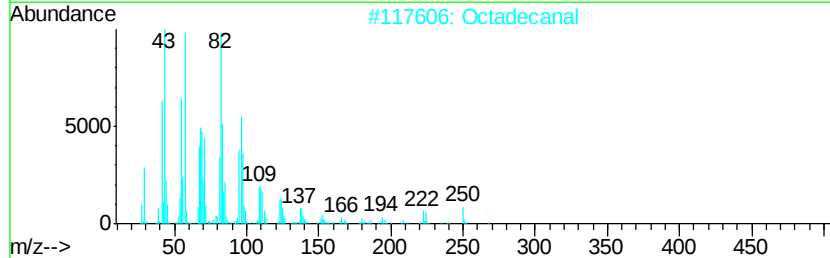
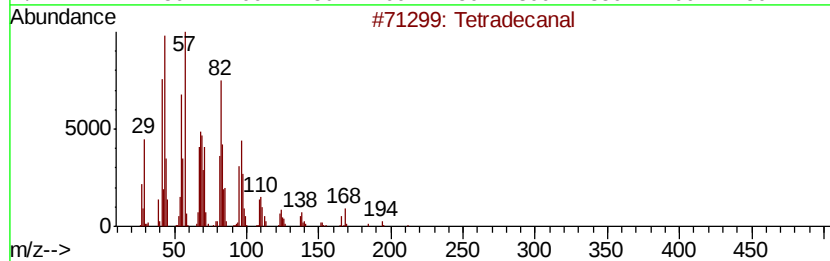
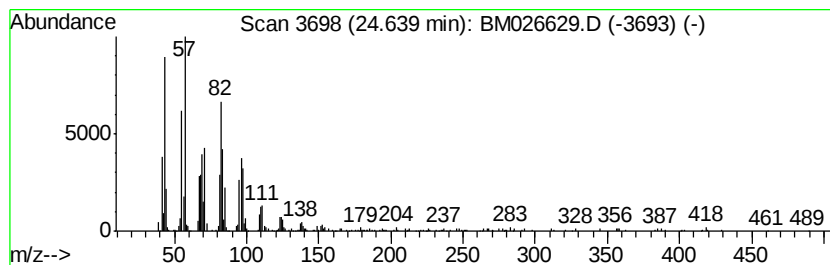
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Tetradecanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.64	6.61 ng	440255	Perylene-d12	23.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanal	212	C14H28O	000124-25-4	91
2			Octadecanal	268	C18H36O	000638-66-4	91
3			Octadecanoic acid, 3-hydroxy-2-t...	511	C33H66O3	018951-36-5	72
4			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	64
5			2-Octadecyl-propane-1,3-diol	328	C21H44O2	005337-61-1	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
Data File : BM026629.D
Acq On : 01 Jul 2020 10:03
Operator : JU/CG
Sample : L3153-34
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SP2-I

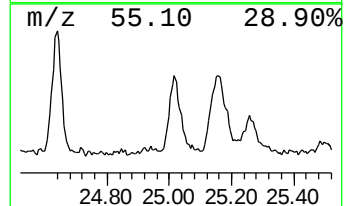
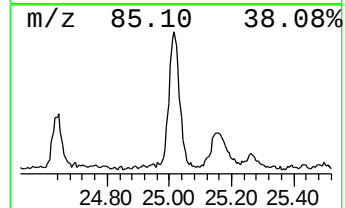
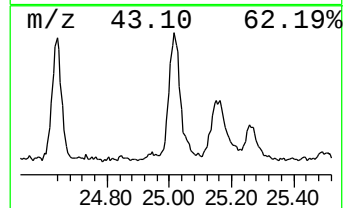
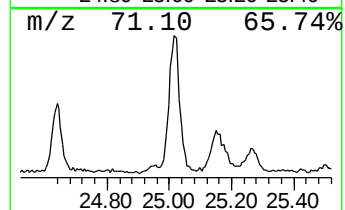
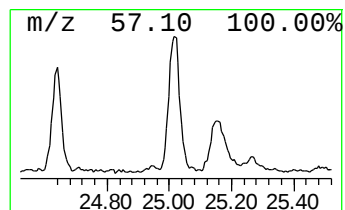
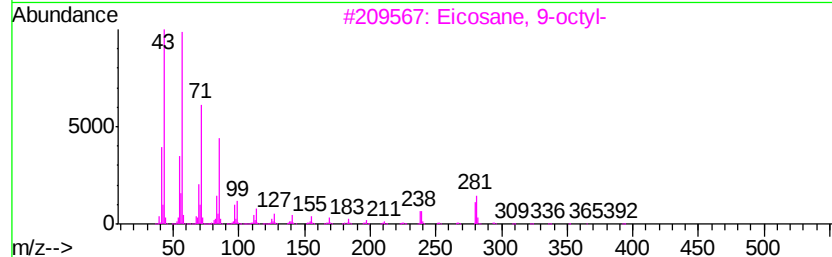
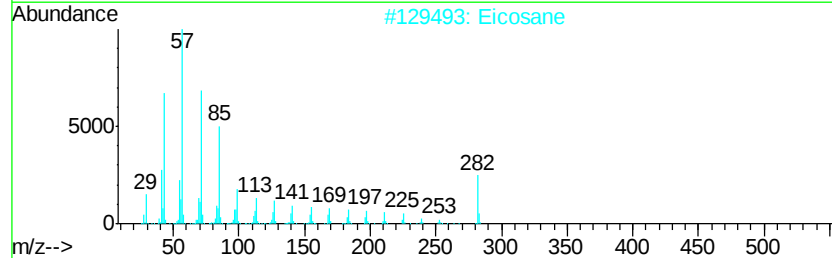
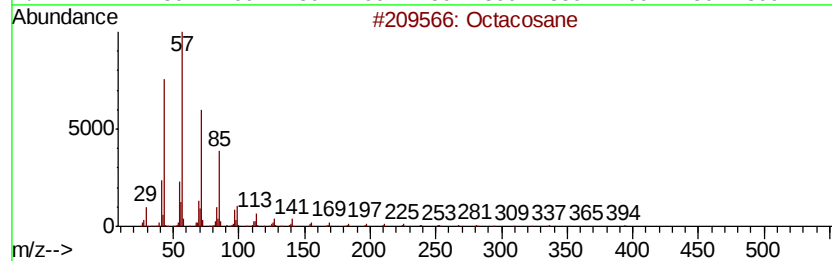
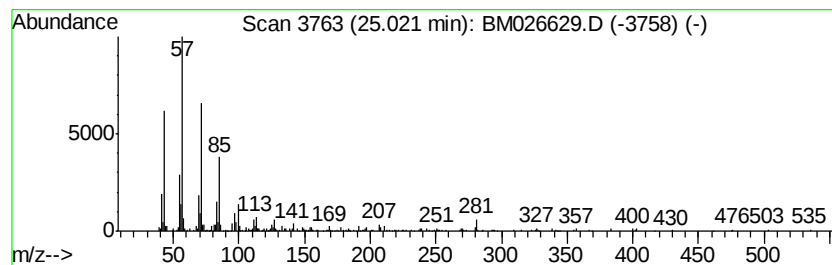
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Octacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.02	5.33 ng	355372	Perylene-d12	23.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	87
2		Eicosane	282	C20H42	000112-95-8	87
3		Eicosane, 9-octyl-	394	C28H58	013475-77-9	83
4		Nonadecane	268	C19H40	000629-92-5	83
5		Docosane	310	C22H46	000629-97-0	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
Data File : BM026629.D
Acq On : 01 Jul 2020 10:03
Operator : JU/CG
Sample : L3153-34
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP2-I

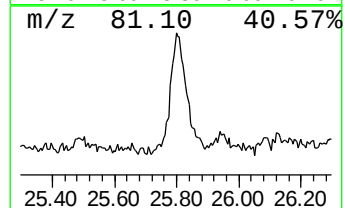
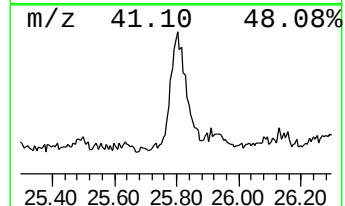
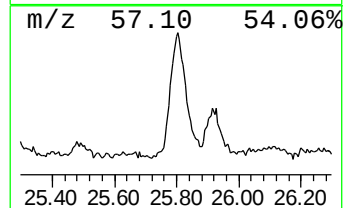
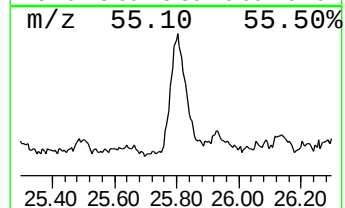
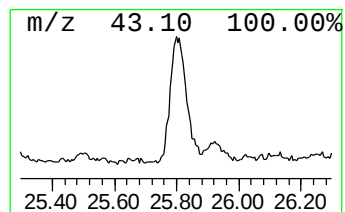
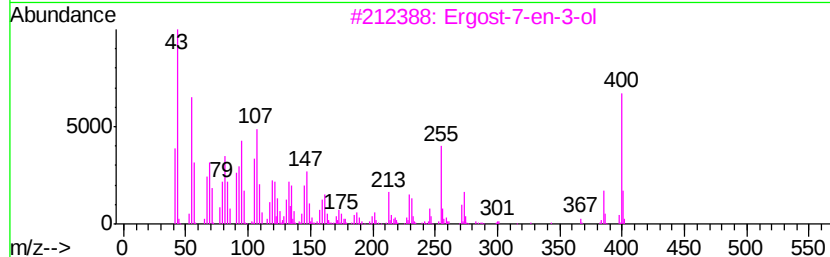
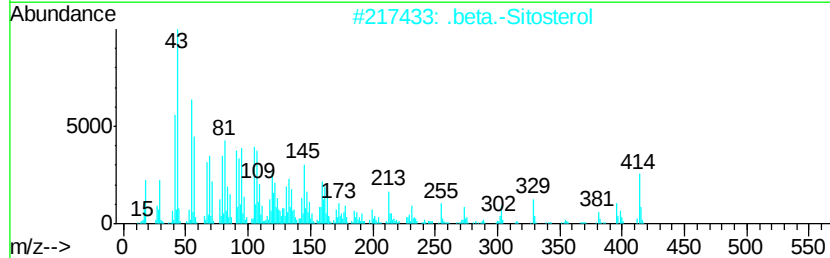
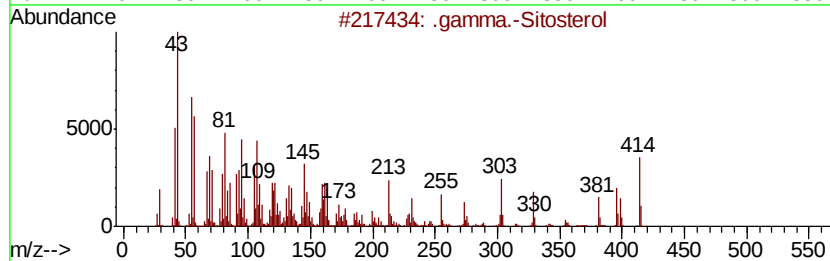
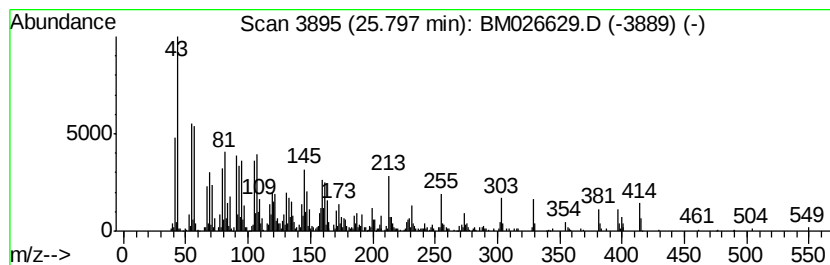
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 .gamma.-Sitosterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.80	13.62 ng	907436	Perylene-d12	23.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	98
3		Ergost-7-en-3-ol	400	C28H48O	116179-22-7	52
4		Methyl (25RS)-3.beta.-hydroxy-5-...	430	C28H46O3	056845-86-4	46
5		Cholest-7-en-3-ol, 4,4-dimethyl-...	414	C29H50O	006384-28-7	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM070120\
 Data File : BM026629.D
 Acq On : 01 Jul 2020 10:03
 Operator : JU/CG
 Sample : L3153-34
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP2-I

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.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
Cinnamyl cinnamate	20.56	2.1 ng		123724	5	20.99	1201030	20.0
5-Eicosene, (E)-	20.74	8.9 ng		534569	5	20.99	1201030	20.0
1-Docosene	21.62	13.1 ng		785614	5	20.99	1201030	20.0
Eicosane	22.03	2.5 ng		163013	6	23.07	1332980	20.0
1,19-Eicosadiene	22.23	2.9 ng		196138	6	23.07	1332980	20.0
Eicosane, 10-methyl-	22.49	21.2 ng		1412130	6	23.07	1332980	20.0
Behenic alcohol	22.53	6.4 ng		429063	6	23.07	1332980	20.0
Tetradecane, 2,6,...	23.00	4.7 ng		311948	6	23.07	1332980	20.0
Oxirane, heptadecyl-	23.28	7.3 ng		489298	6	23.07	1332980	20.0
Heptadecane, 9-he...	23.58	23.4 ng		1557030	6	23.07	1332980	20.0
Octacosanol	23.66	6.9 ng		458699	6	23.07	1332980	20.0
Tetradecanal	24.64	6.6 ng		440255	6	23.07	1332980	20.0
Octacosane	25.02	5.3 ng		355372	6	23.07	1332980	20.0
.gamma.-Sitosterol	25.80	13.6 ng		907436	6	23.07	1332980	20.0