

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022620\
 Data File : BG044605.D
 Acq On : 26 Feb 2020 16:02
 Operator : CG/JU
 Sample : PB127106BL
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB127106BL

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_G\METHODS\8270-BG022420.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	5.449	396	402	415	rBV	371075	612887	12.60%	2.538%
2	7.048	667	674	695	rBV	205652	391261	8.04%	1.620%
3	7.870	807	814	822	rBV	191676	330572	6.80%	1.369%
4	8.193	862	869	879	rBV	814572	1409398	28.98%	5.836%
5	9.028	1003	1011	1028	rBV	612331	1171632	24.09%	4.851%
6	9.362	1035	1068	1088	rBV2	613793	3684832	75.76%	15.258%
7	10.673	1283	1291	1301	rBV	267180	494215	10.16%	2.046%
8	11.542	1431	1439	1448	rBV3	19972	65265	1.34%	0.270%
9	12.406	1579	1586	1603	rBV	264400	454042	9.34%	1.880%
10	13.135	1703	1710	1718	rBV	1894888	2962218	60.90%	12.265%
11	13.975	1846	1853	1864	rBV	31459	55147	1.13%	0.228%
12	14.515	1938	1945	1954	rBV	485211	771316	15.86%	3.194%
13	15.250	2061	2070	2083	rBV3	12249	49653	1.02%	0.206%
14	16.002	2191	2198	2211	rBV	1571827	2449263	50.36%	10.141%
15	17.259	2405	2412	2420	rBV	631667	975983	20.07%	4.041%
16	19.880	2851	2858	2869	rBV	3504481	4863793	100.00%	20.139%
17	21.166	3072	3077	3088	rBV2	183743	310239	6.38%	1.285%
18	21.501	3127	3134	3149	rBV	641478	1101599	22.65%	4.561%
19	21.701	3164	3168	3173	rBV3	53342	72042	1.48%	0.298%
20	22.283	3262	3267	3277	rVB	77139	135993	2.80%	0.563%
21	22.606	3318	3322	3331	rBV4	22595	57372	1.18%	0.238%
22	22.941	3374	3379	3386	rBV	85567	155333	3.19%	0.643%
23	23.704	3503	3509	3517	rVB	85486	177888	3.66%	0.737%
24	24.562	3646	3655	3672	rBV	400744	1260621	25.92%	5.220%
25	25.667	3836	3843	3852	rVB4	48955	138353	2.84%	0.573%

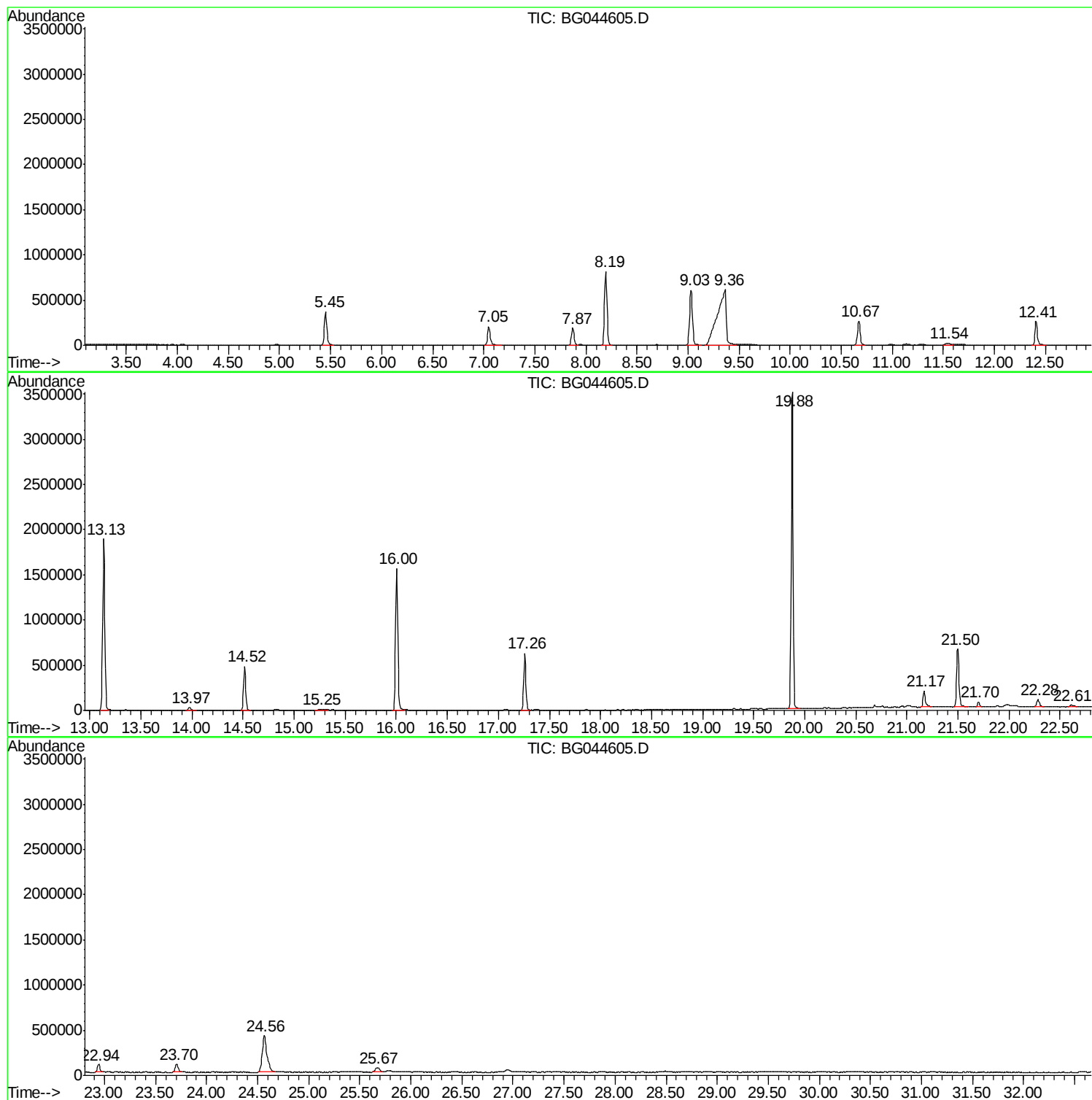
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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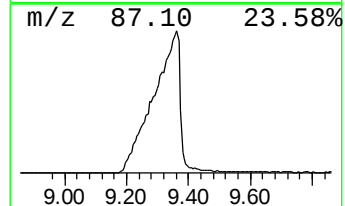
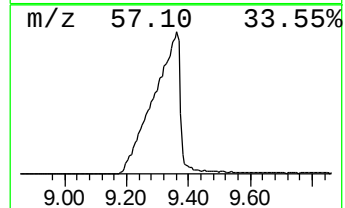
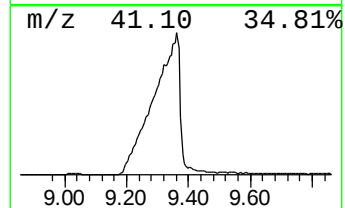
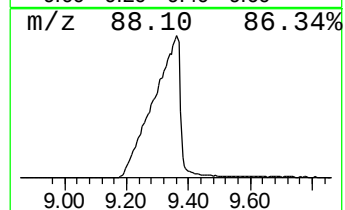
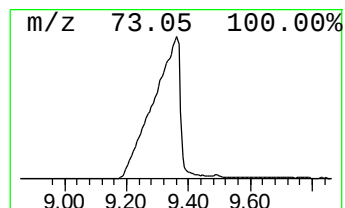
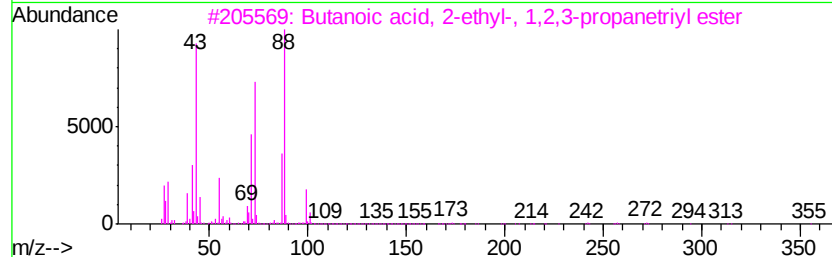
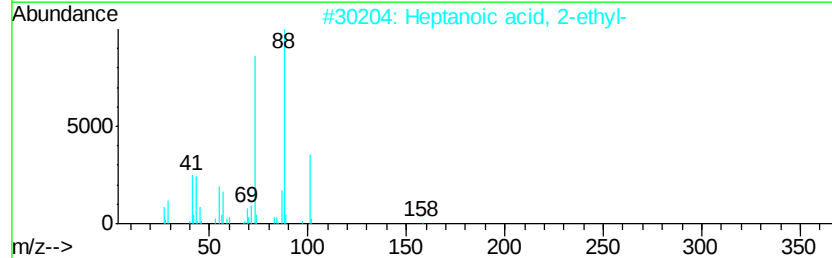
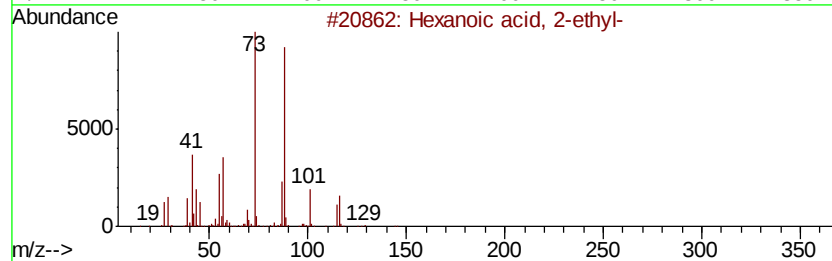
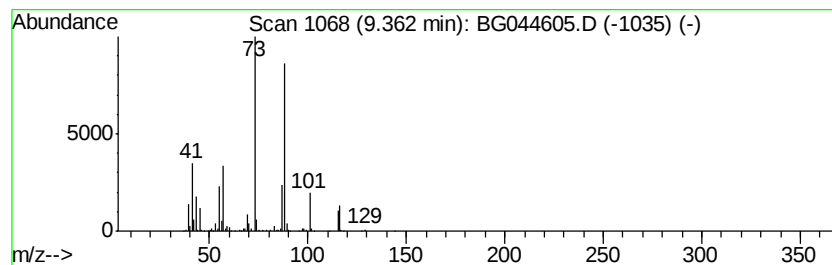
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.36	149.12 ng	3684830	Naphthalene-d8	10.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
3		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	50
4		Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	42
5		Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	40



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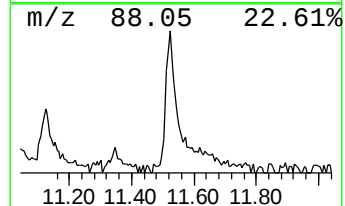
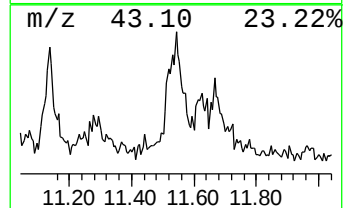
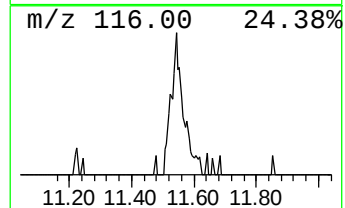
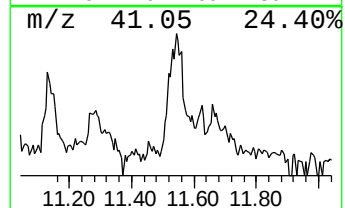
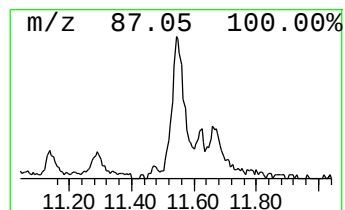
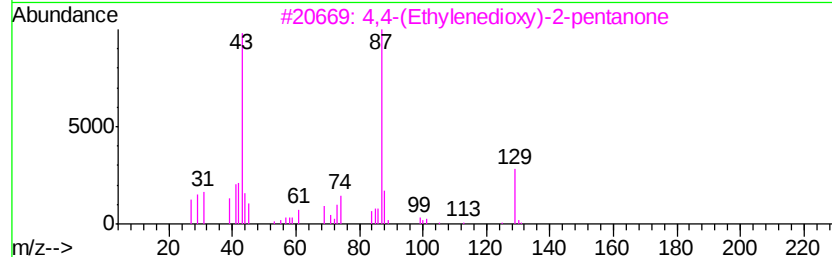
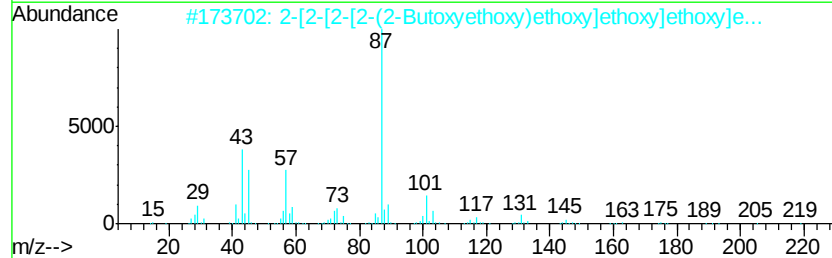
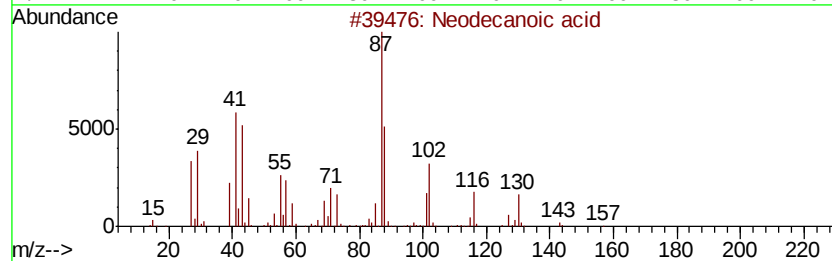
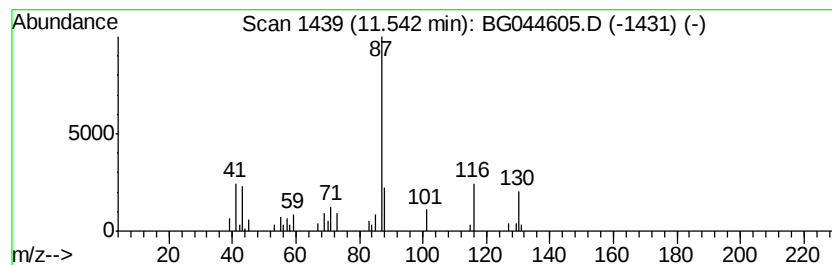
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Peak Number 3 unknown11.54 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	2.64 ng	65265	Naphthalene-d8	10.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Neodecanoic acid	172	C10H20O2	026896-20-8	47
2		2-[2-[2-[2-(2-Butoxyethoxy)ethoxy]ethoxy]ethoxy]e...	336	C16H32O7	1000351-94-0	47
3		4,4-(Ethylenedioxy)-2-pentanone	144	C7H12O3	014255-36-8	47
4		Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	47
5		3,4-Di-O-methyl-L-arabinopyranose	178	C7H14O5	086049-20-9	42



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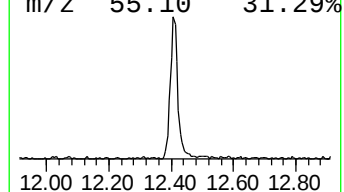
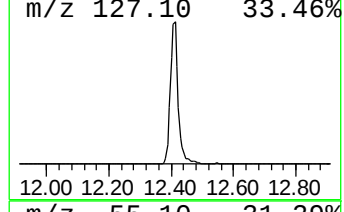
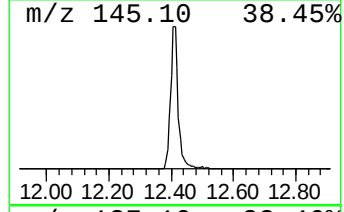
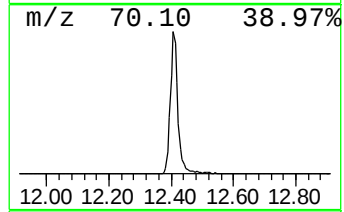
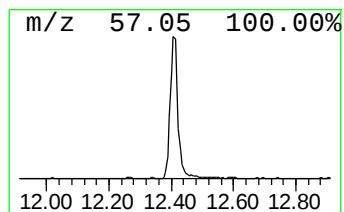
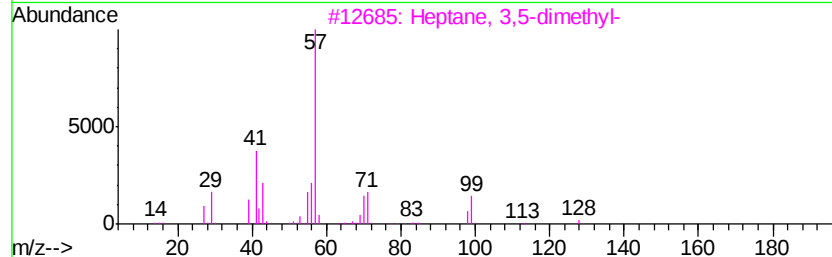
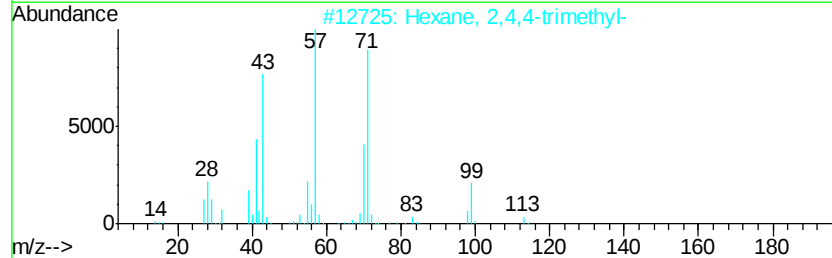
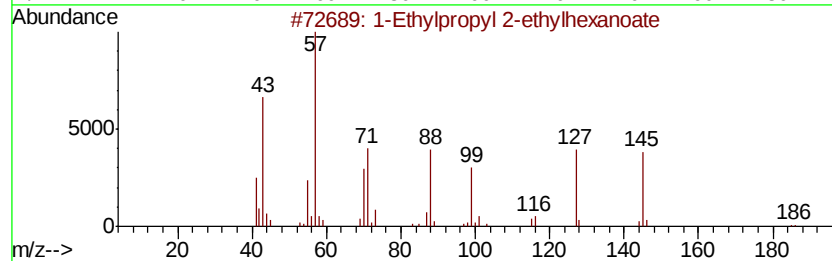
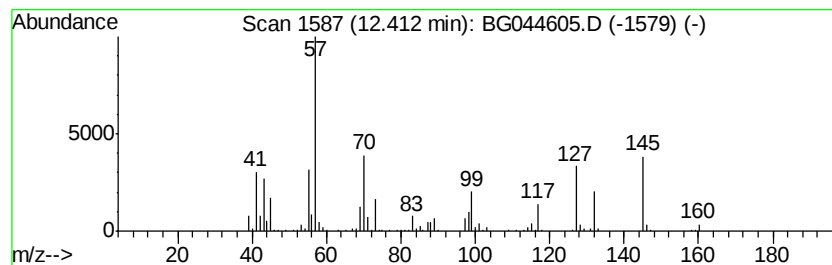
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Peak Number 4 unknown12.41 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.41	18.37 ng	454042	Naphthalene-d8	10.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Ethylpropyl 2-ethylhexanoate	214	C13H26O2	1000099-98-7	38
2		Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	32
3		Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	22
4		1-Pentanol, 2,2,4-trimethyl-	130	C8H18O	000123-44-4	22
5		1-Butanol, 2-methyl-, propanoate	144	C8H16O2	002438-20-2	22



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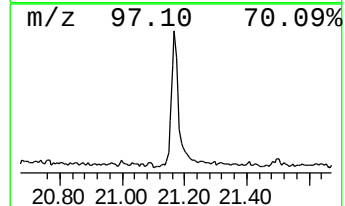
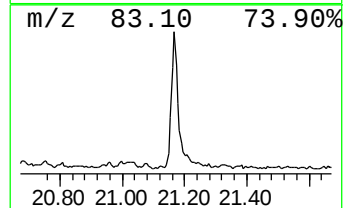
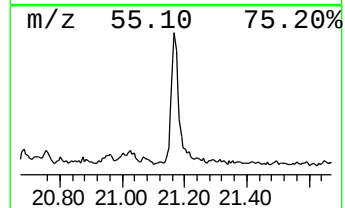
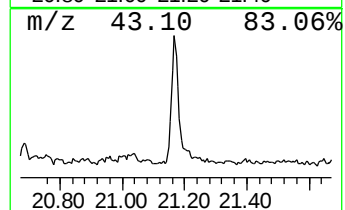
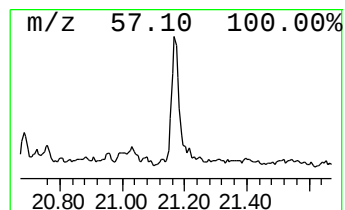
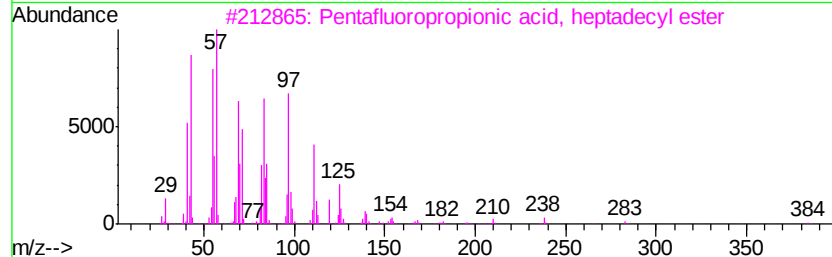
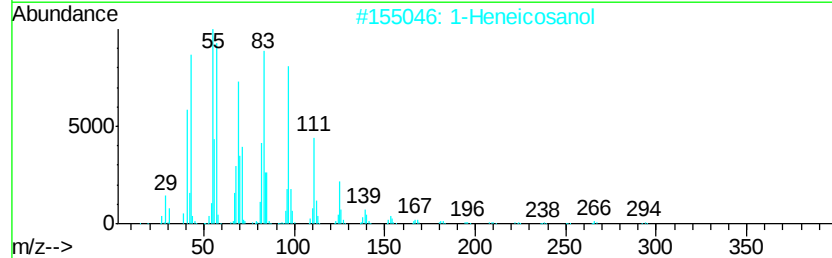
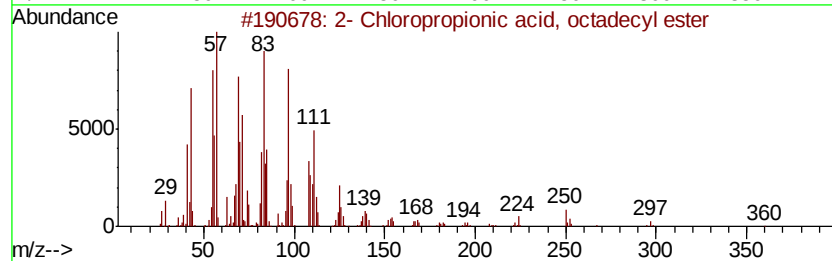
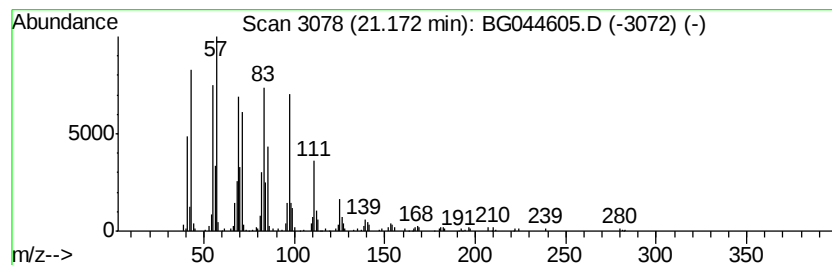
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Peak Number 5 2- Chloropropionic acid, oc... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.17	5.63 ng	310239	Chrysene-d12	21.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	93
4		Behenic alcohol	326	C22H46O	000661-19-8	93
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93



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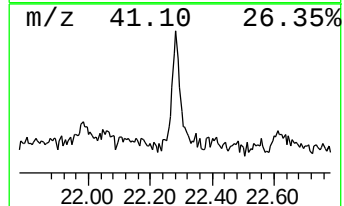
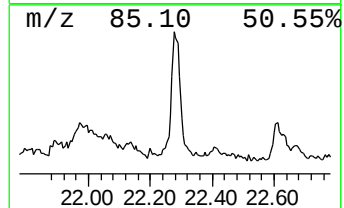
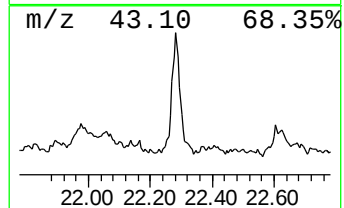
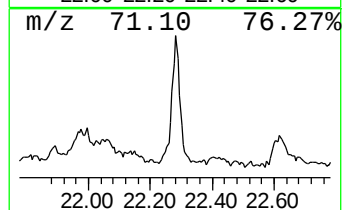
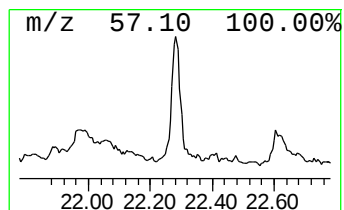
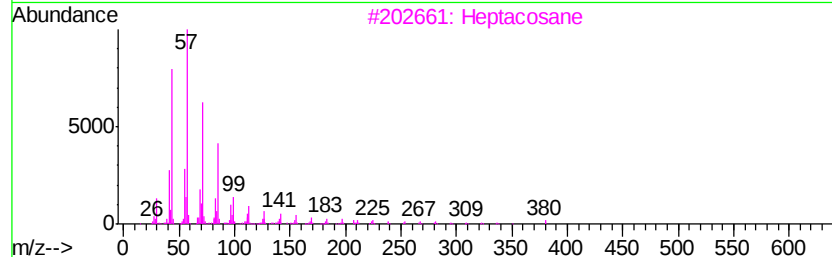
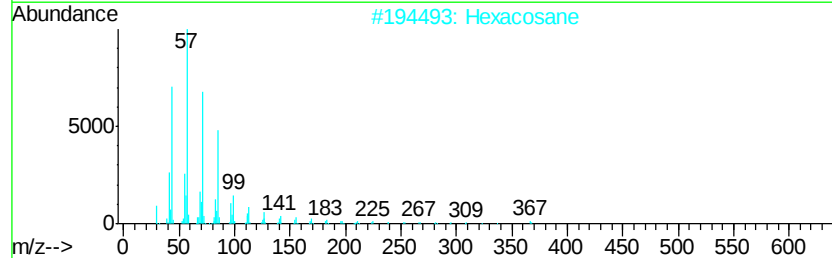
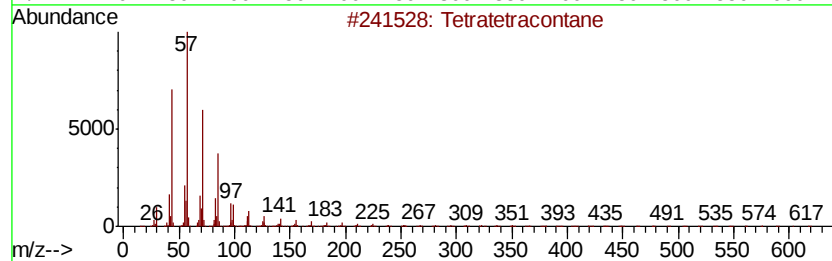
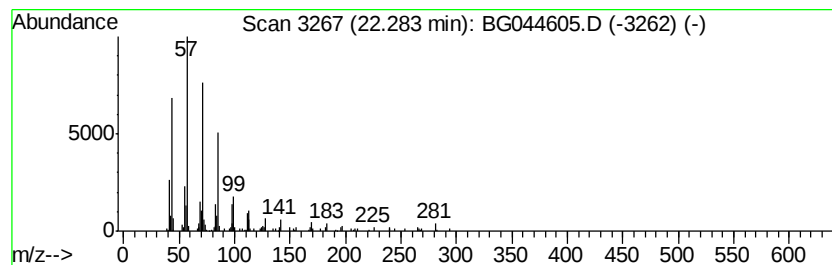
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Peak Number 6 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	2.47 ng	135993	Chrysene-d12	21.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Heptadecane	240	C17H36	000629-78-7	91
5		Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	91



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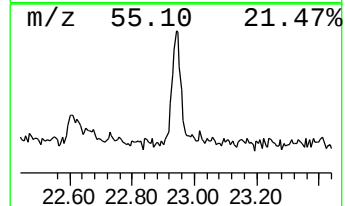
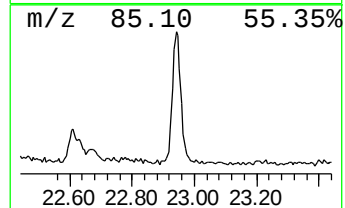
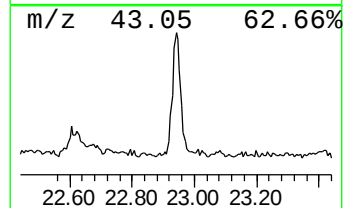
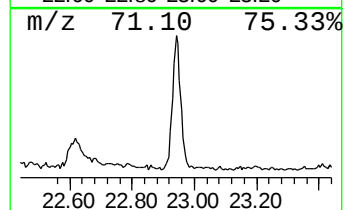
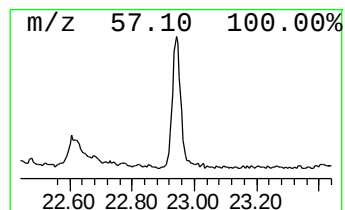
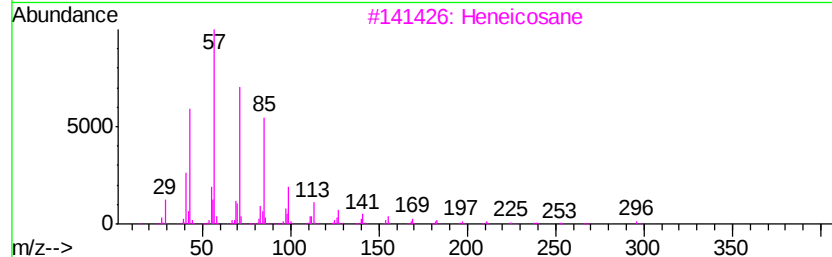
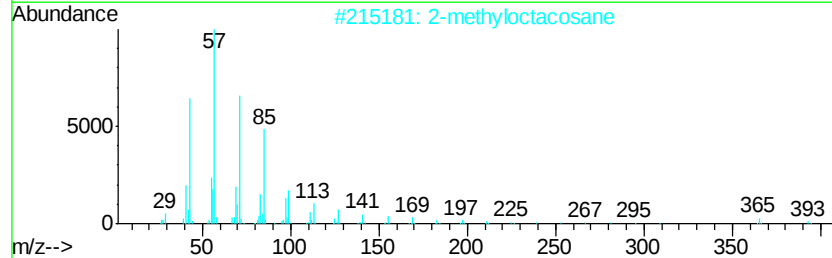
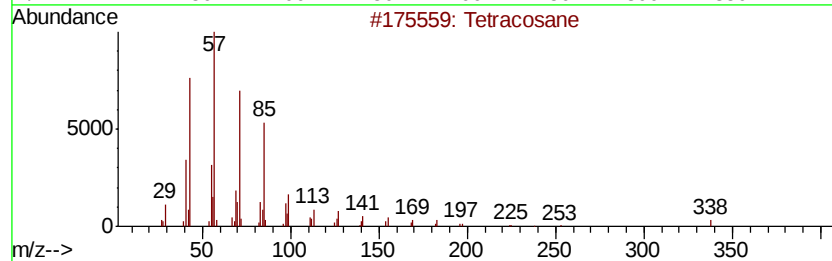
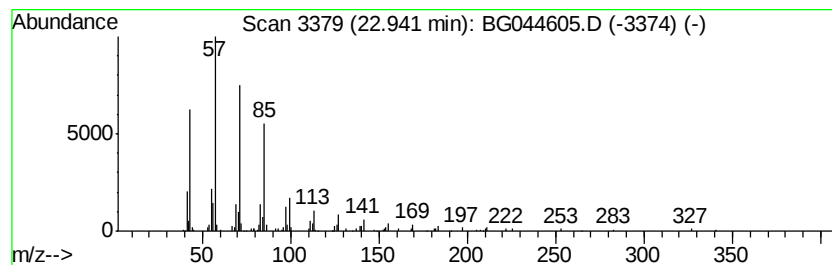
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.94	2.82 ng	155333	Chrysene-d12	21.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022620\
Data File : BG044605.D
Acq On : 26 Feb 2020 16:02
Operator : CG/JU
Sample : PB127106BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB127106BL

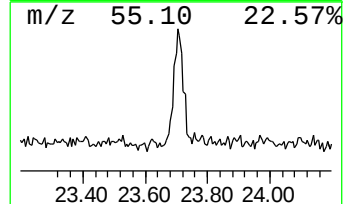
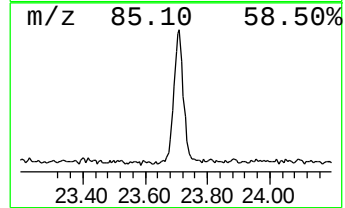
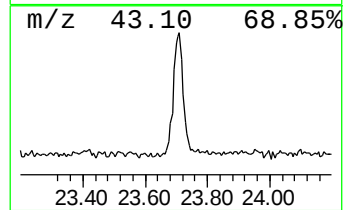
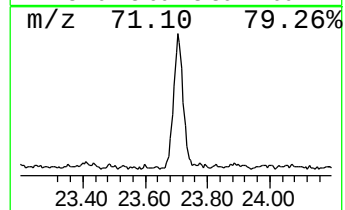
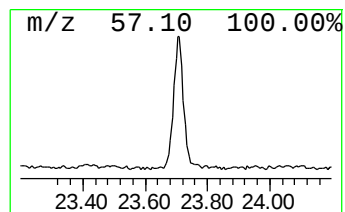
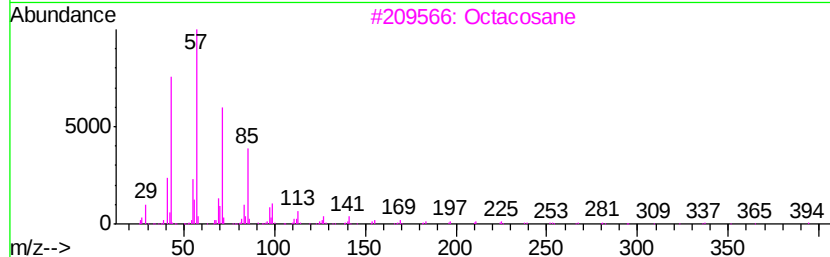
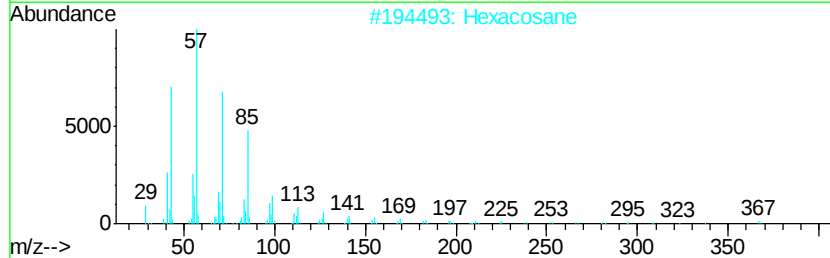
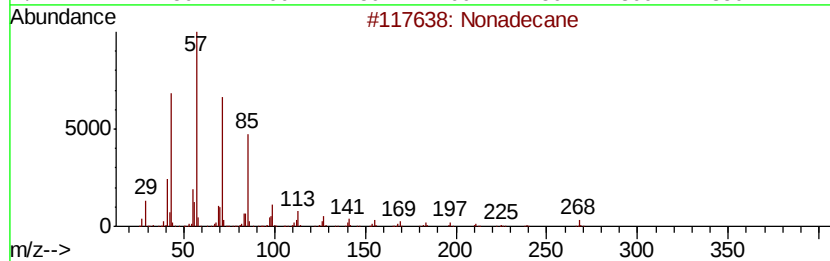
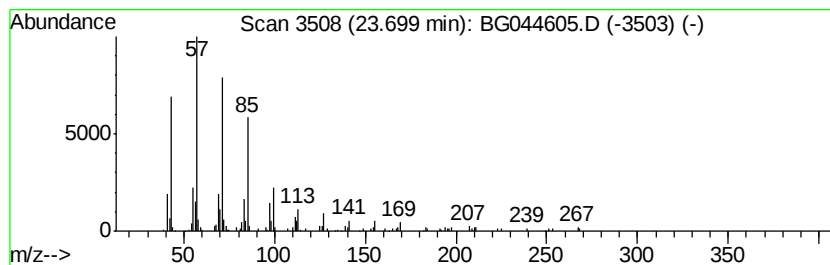
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.70	2.82 ng	177888	Perylene-d12	24.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	93
2		Hexacosane	366	C26H54	000630-01-3	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022620\
Data File : BG044605.D
Acq On : 26 Feb 2020 16:02
Operator : CG/JU
Sample : PB127106BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB127106BL

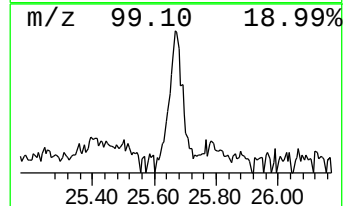
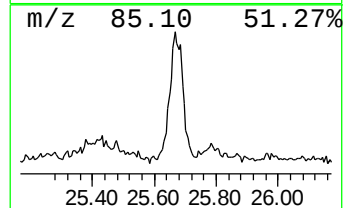
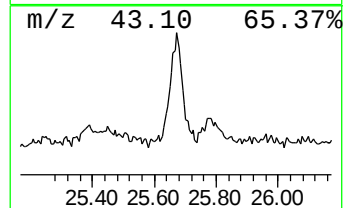
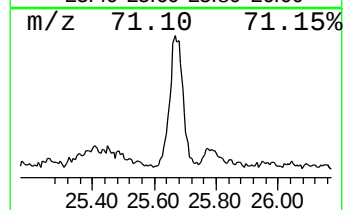
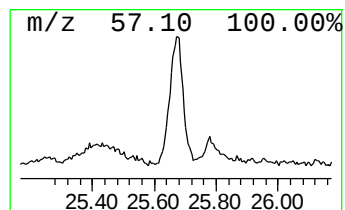
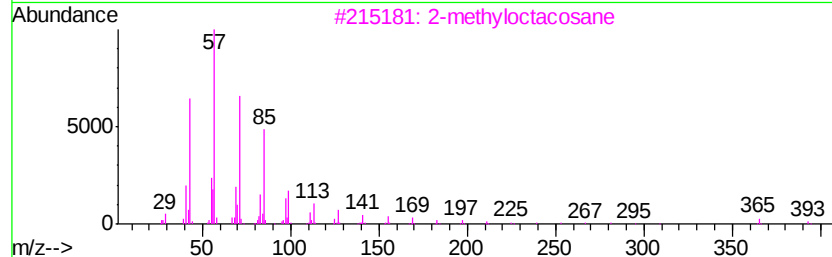
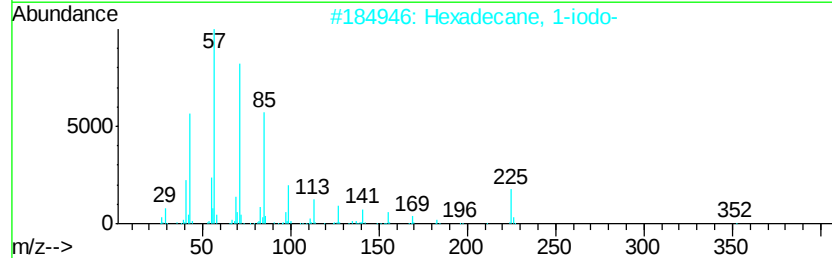
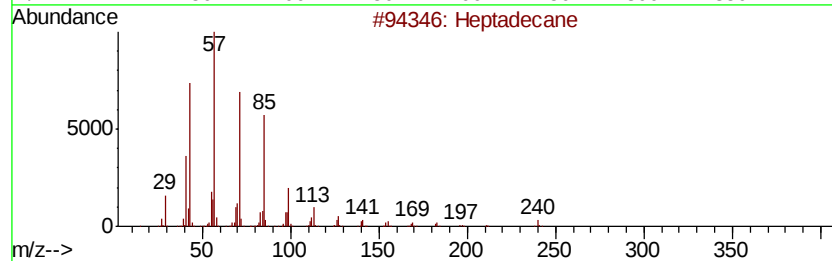
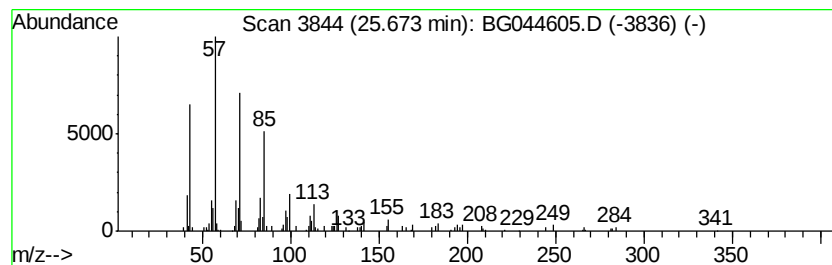
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG022420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.67	2.20 ng	138353	Perylene-d12	24.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Hexadecane, 1-iodo-		352	C16H33I	000544-77-4	87
3	2-methyloctacosane		408	C29H60	1000376-72-8	87
4	Hexadecane		226	C16H34	000544-76-3	87
5	Heneicosane		296	C21H44	000629-94-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG022620\
Data File : BG044605.D
Acq On : 26 Feb 2020 16:02
Operator : CG/JU
Sample : PB127106BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB127106BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG022420.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
Hexanoic acid, 2-...	9.36	149.1	ng	3684830	2	10.67	494215	20.0
unknown11.54	11.54	2.6	ng	65265	2	10.67	494215	20.0
unknown12.41	12.41	18.4	ng	454042	2	10.67	494215	20.0
2- Chloropropioni...	21.17	5.6	ng	310239	5	21.50	1101600	20.0
Tetratetracontane	22.28	2.5	ng	135993	5	21.50	1101600	20.0
Tetracosane	22.94	2.8	ng	155333	5	21.50	1101600	20.0
Nonadecane	23.70	2.8	ng	177888	6	24.56	1260620	20.0
Heptadecane	25.67	2.2	ng	138353	6	24.56	1260620	20.0