

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG021720\
 Data File : BG044459.D
 Acq On : 17 Feb 2020 22:55
 Operator : CG/JU
 Sample : L1547-15
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MARCY-GREEN-BH-03-C

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-BG013020.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	4.991	319	324	333	rVB2	28904	47706	1.38%	0.211%
2	5.473	398	406	423	rBV	868559	1462660	42.34%	6.461%
3	7.065	669	677	695	rBV	852177	1528152	44.24%	6.750%
4	7.887	811	817	826	rBV	252763	431742	12.50%	1.907%
5	8.211	864	872	882	rBV	722373	1278937	37.02%	5.649%
6	9.045	1006	1014	1027	rBV	522981	965010	27.94%	4.263%
7	10.690	1285	1294	1310	rBV	313131	605645	17.53%	2.675%
8	13.152	1705	1713	1723	rBV	1397253	2307403	66.80%	10.192%
9	13.986	1849	1855	1867	rBV	39299	66386	1.92%	0.293%
10	14.527	1940	1947	1954	rBV	532286	847614	24.54%	3.744%
11	16.019	2194	2201	2213	rBV	1060128	1695652	49.09%	7.490%
12	16.589	2294	2298	2303	rVB2	44086	60063	1.74%	0.265%
13	17.271	2407	2414	2419	rBV	690902	1068860	30.94%	4.721%
14	17.312	2419	2421	2429	rVV	172353	234991	6.80%	1.038%
15	17.406	2432	2437	2445	rVB	24004	40752	1.18%	0.180%
16	18.152	2559	2564	2568	rBV	29765	49311	1.43%	0.218%
17	18.199	2568	2572	2577	rVB	39308	57370	1.66%	0.253%
18	18.340	2591	2596	2600	rBV2	37119	70942	2.05%	0.313%
19	18.381	2600	2603	2608	rVB	24366	36236	1.05%	0.160%
20	19.327	2758	2764	2771	rVB	221522	318495	9.22%	1.407%
21	19.685	2815	2825	2834	rBV	215892	370657	10.73%	1.637%
22	19.891	2851	2860	2874	rVB	2580527	3454268	100.00%	15.258%
23	20.338	2930	2936	2940	rBV2	25857	41828	1.21%	0.185%
24	20.931	3033	3037	3043	rVB	24195	38212	1.11%	0.169%
25	21.107	3060	3067	3071	rBV3	23192	55008	1.59%	0.243%
26	21.184	3075	3080	3088	rVV2	231116	379172	10.98%	1.675%
27	21.513	3128	3136	3141	rBV	802940	1405605	40.69%	6.209%
28	21.560	3141	3144	3157	rVB	104889	171879	4.98%	0.759%
29	21.718	3166	3171	3178	rVB3	45609	71488	2.07%	0.316%
30	22.312	3265	3272	3282	rBV4	79640	209335	6.06%	0.925%
31	22.964	3378	3383	3391	rVB	74175	137292	3.97%	0.606%
32	23.293	3436	3439	3448	rVB8	20513	39269	1.14%	0.173%
33	23.622	3487	3495	3502	rBV2	61622	196845	5.70%	0.869%
34	23.734	3509	3514	3520	rBV	85886	168205	4.87%	0.743%

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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

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35	23.792	3520	3524	3533	rVB3	32307	64484	1.87%	0.285%
36	24.303	3605	3611	3622	rVB3	38065	109571	3.17%	0.484%
37	24.439	3628	3634	3646	rVB	53913	146727	4.25%	0.648%
38	24.591	3649	3660	3680	rBV2	453971	1488117	43.08%	6.573%
39	25.708	3840	3850	3861	rBV4	72188	217077	6.28%	0.959%
40	25.825	3864	3870	3878	rBV7	24908	71262	2.06%	0.315%
41	26.994	4063	4069	4080	rVB5	23535	73752	2.14%	0.326%
42	28.064	4243	4251	4252	rBV3	17294	39602	1.15%	0.175%
43	28.575	4319	4338	4352	rBV3	99161	515670	14.93%	2.278%

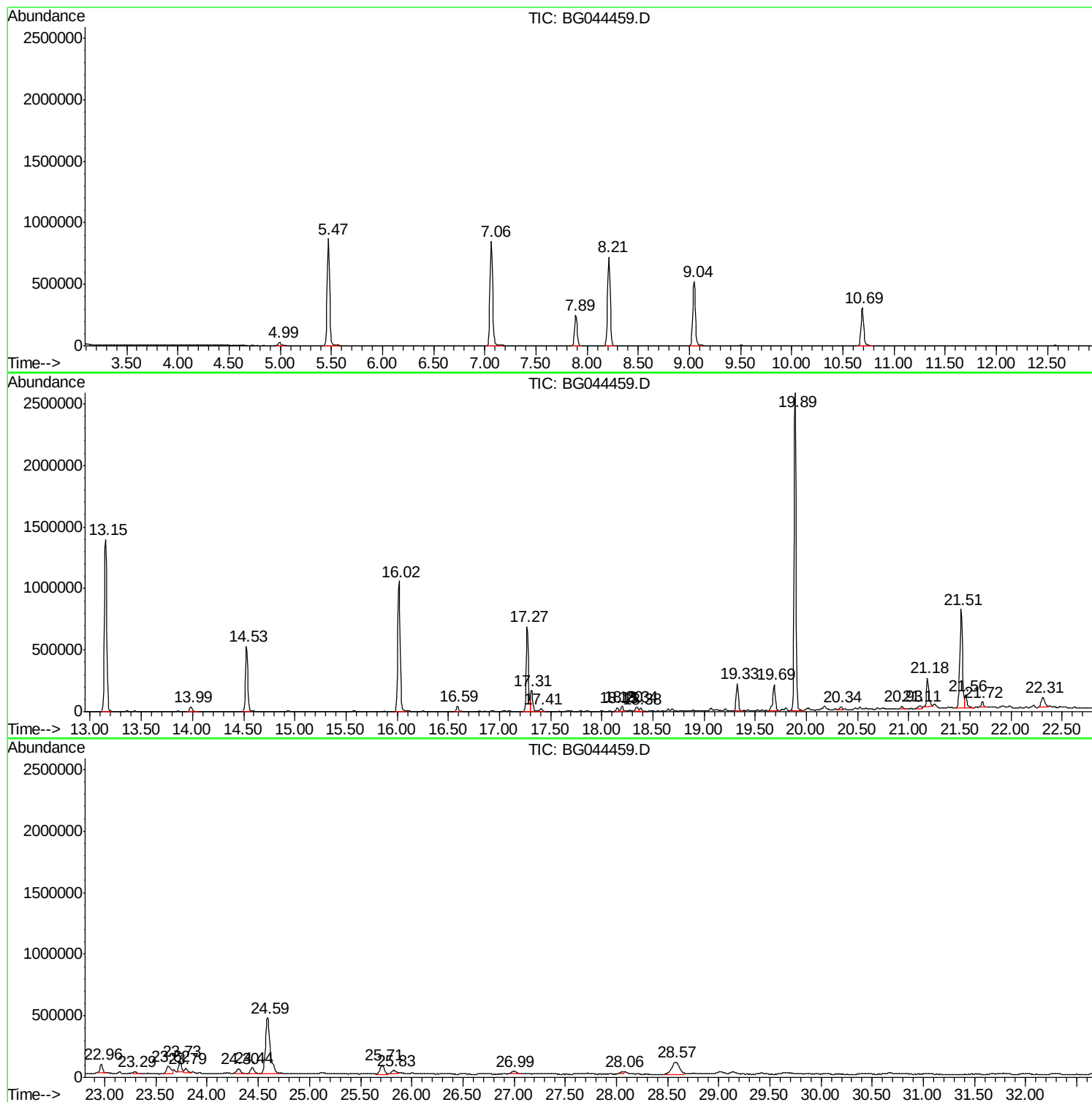
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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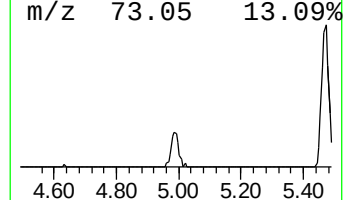
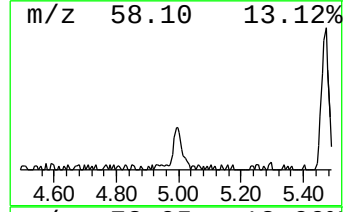
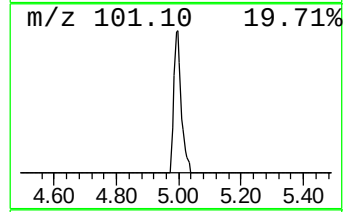
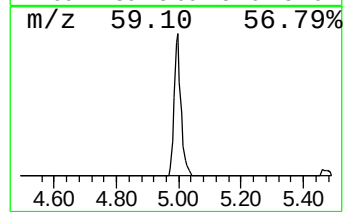
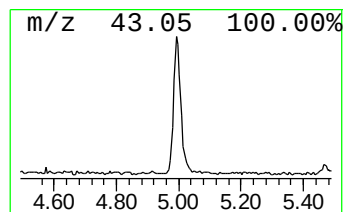
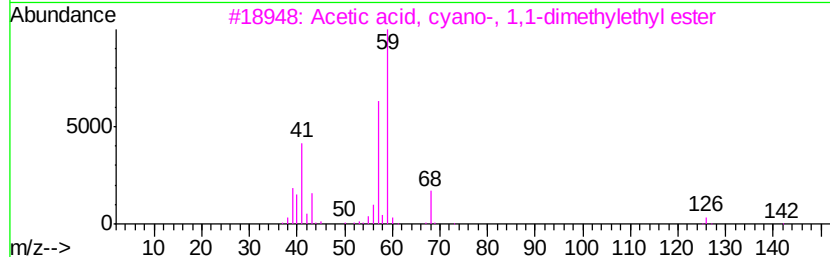
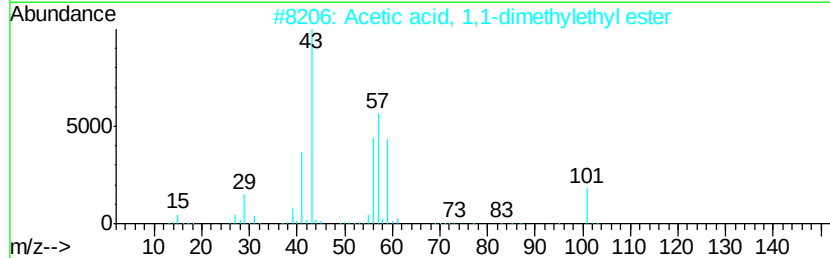
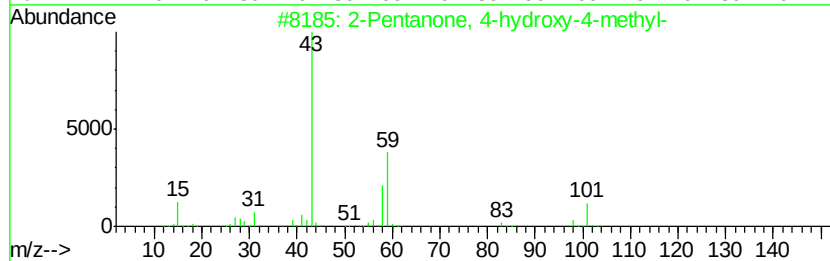
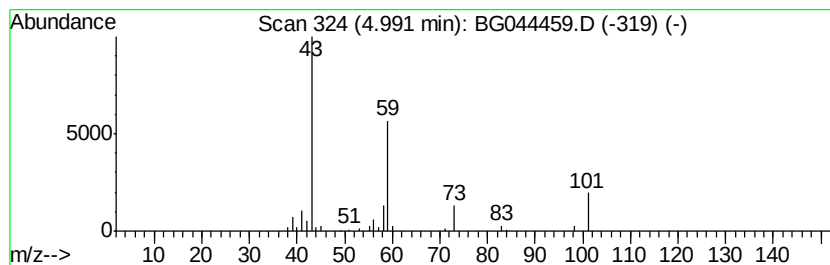
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	2.21 ng	47706	1,4-Dichlorobenzene-d4	7.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	12
5			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10



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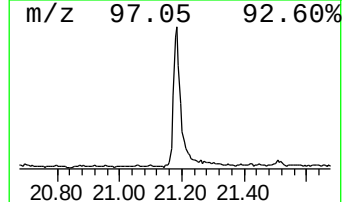
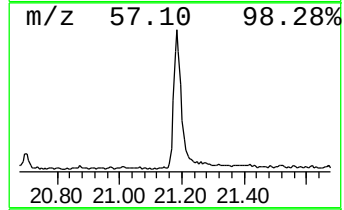
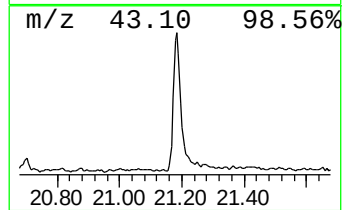
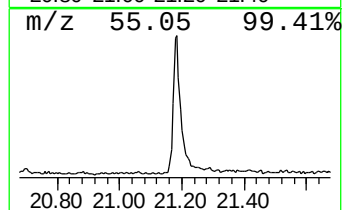
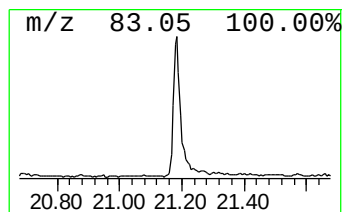
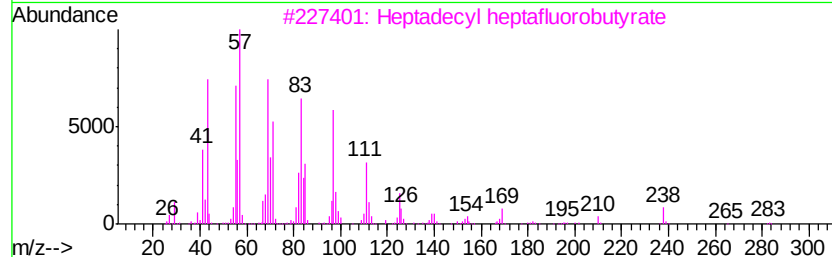
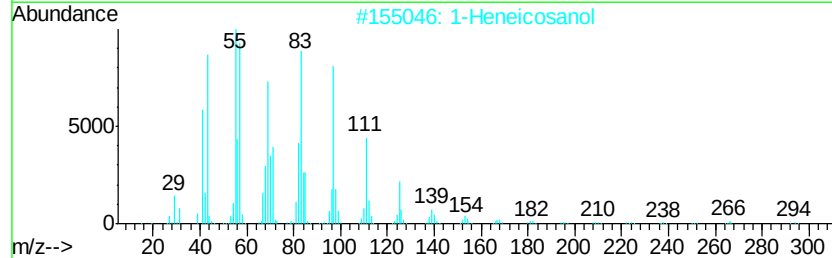
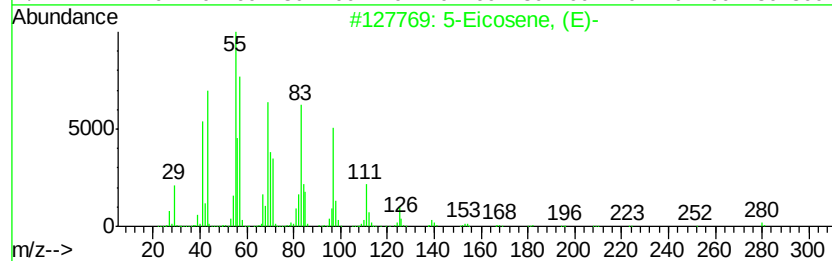
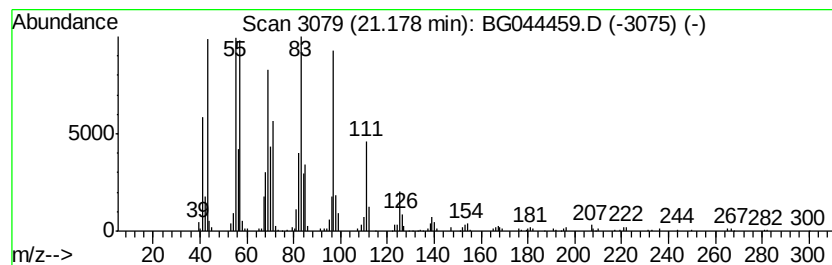
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Peak Number 3 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.18	5.40 ng	379172	Chrysene-d12	21.51	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	1-Nonadecene	266	C19H38	018435-45-5	91



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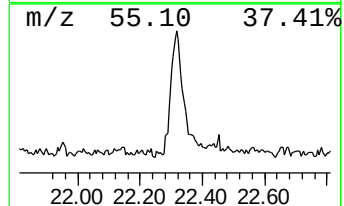
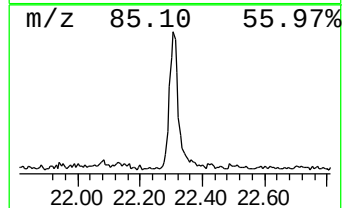
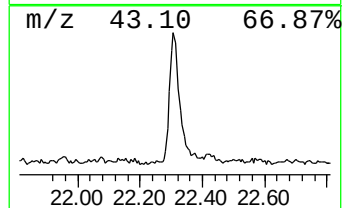
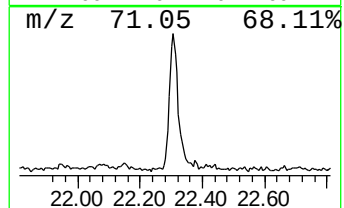
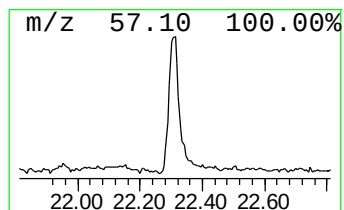
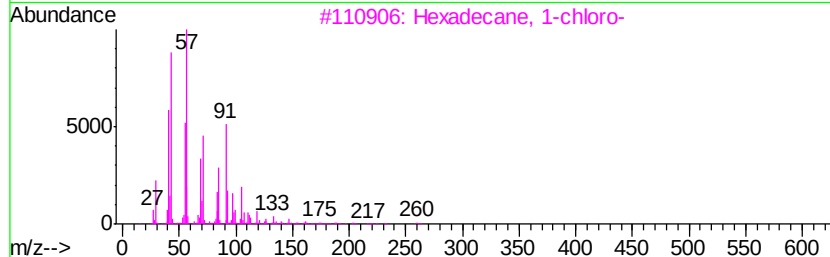
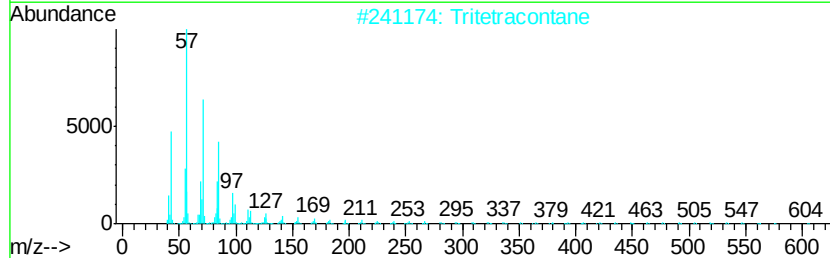
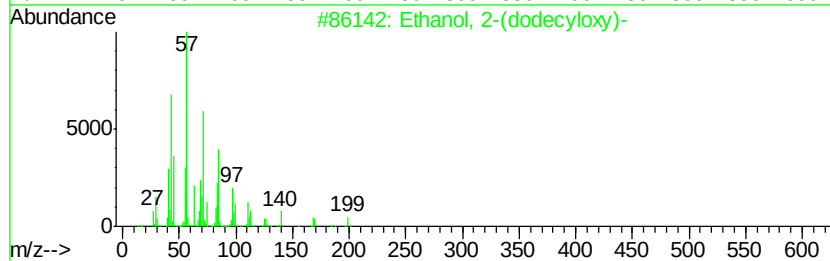
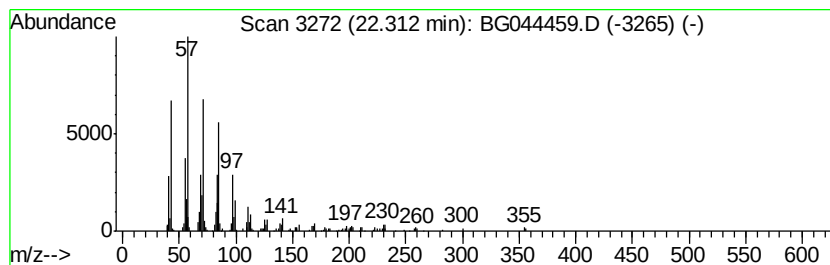
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ClientSampleId :
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 Ethanol, 2-(dodecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
22.31	2.98 ng	209335	Chrysene-d12	21.51		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	90
2		Tritetracontane	605	C43H88	007098-21-7	87
3		Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	83
4		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	74
5		Hexacosane	366	C26H54	000630-01-3	74



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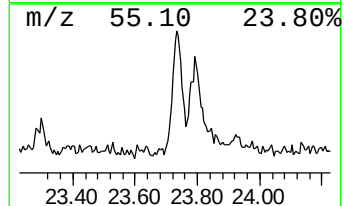
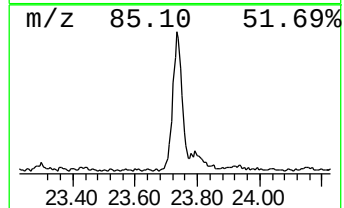
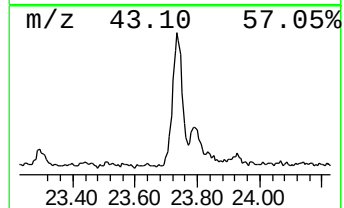
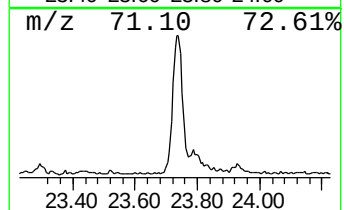
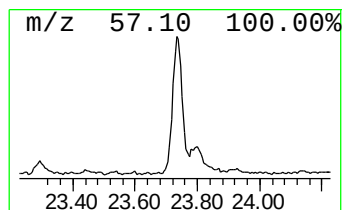
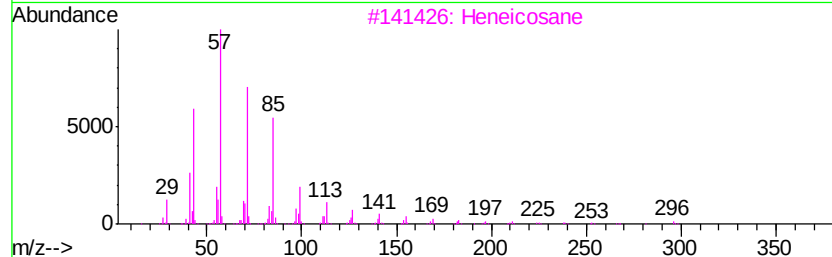
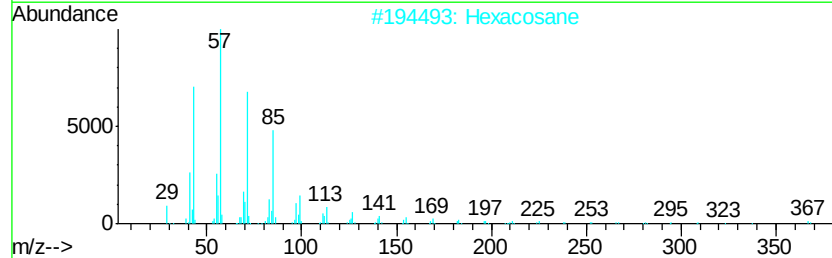
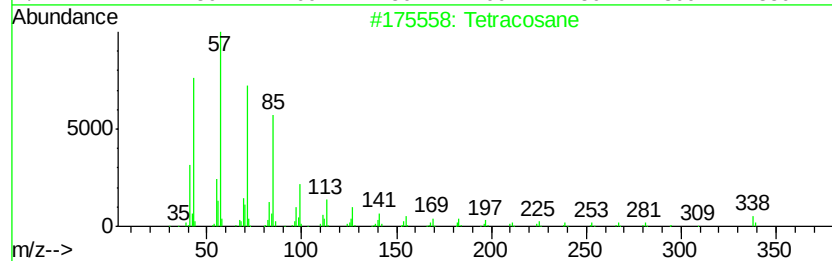
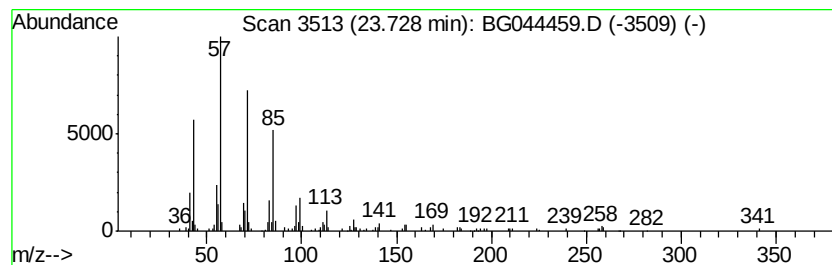
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.73	2.26 ng	168205	Perylene-d12	24.59

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	91
2		Hexacosane	366	C26H54	000630-01-3	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Docosane	310	C22H46	000629-97-0	87
5		Nonadecane	268	C19H40	000629-92-5	87



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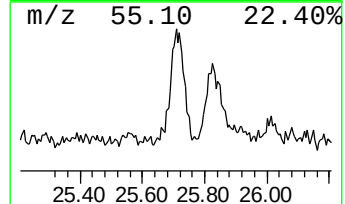
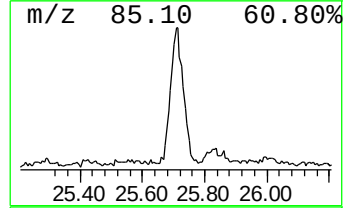
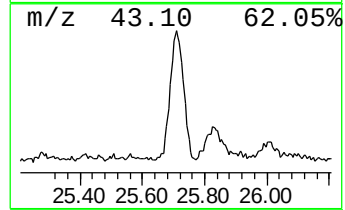
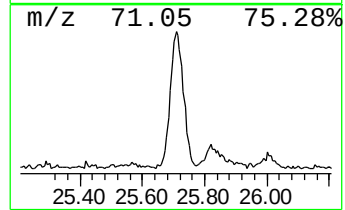
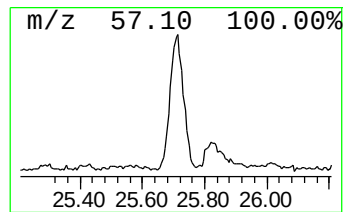
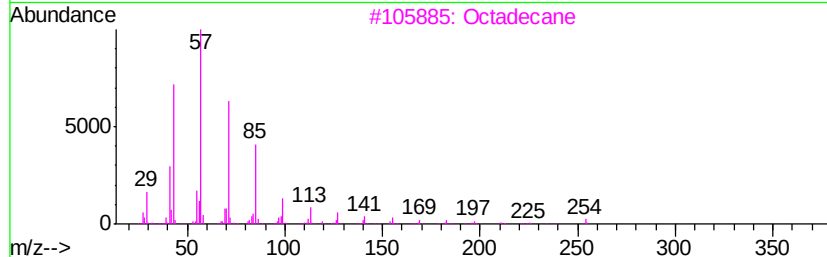
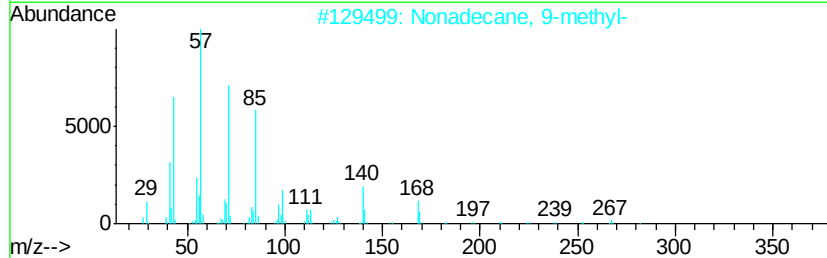
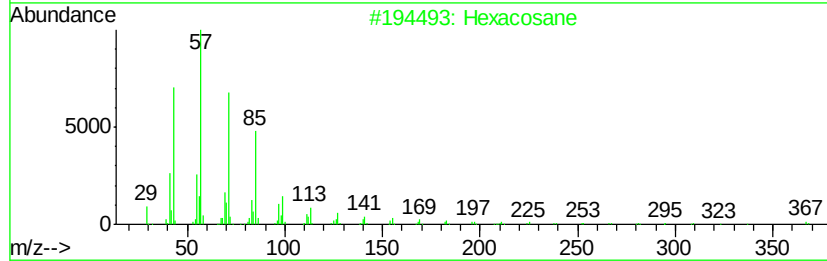
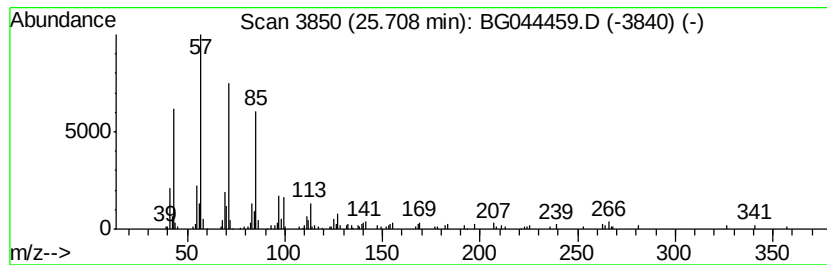
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.71	2.92 ng	217077	Perylene-d12	24.59

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Nonadecane, 9-methyl-		282	C20H42	013287-24-6	90
3	Octadecane		254	C18H38	000593-45-3	87
4	Triacontane		422	C30H62	000638-68-6	87
5	Heneicosane		296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG021720\
Data File : BG044459.D
Acq On : 17 Feb 2020 22:55
Operator : CG/JU
Sample : L1547-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

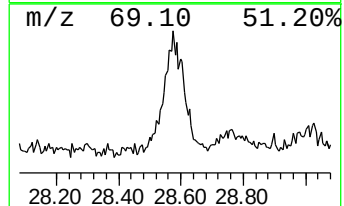
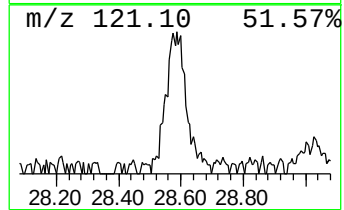
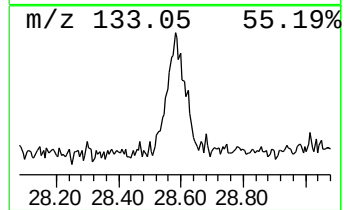
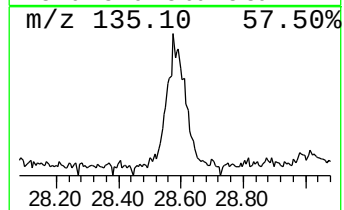
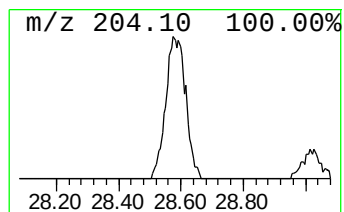
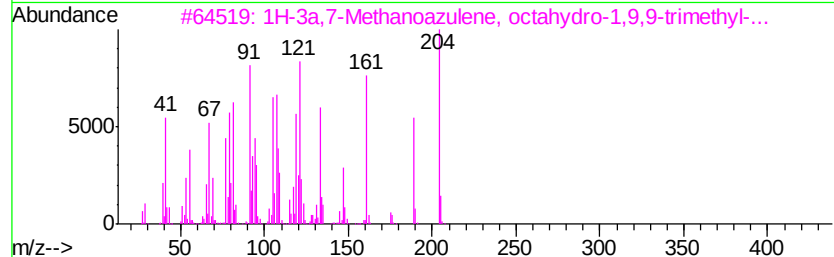
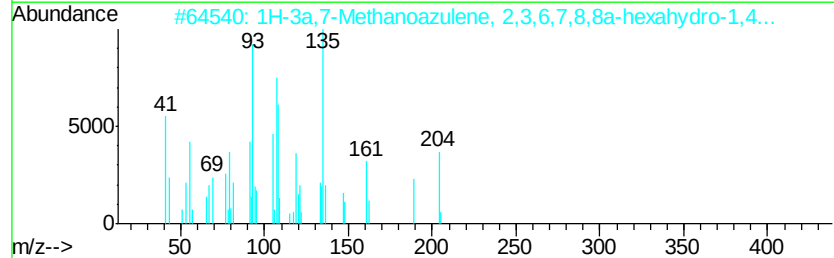
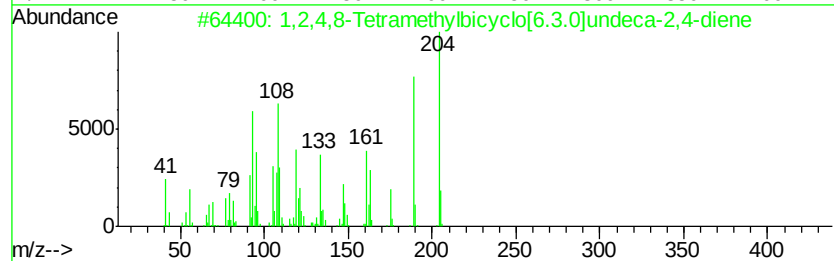
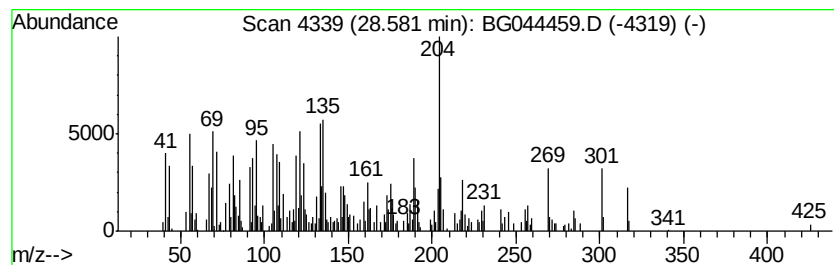
Instrument :
BNA_G
ClientSampleId :
MARCY-GREEN-BH-03-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,2,4,8-Tetramethylbicyclo[...] Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
28.58	6.93 ng	515670	Perylene-d12	24.59	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,8-Tetramethylbicyclo[6.3.0]undeca-2,4-diene	204	C15H24	137235-51-9	78
2	1H-3a,7-Methanoazulene, 2,3,6,7,8a-hexahydro-1,4-dimethyl-	204	C15H24	000560-32-7	78
3	1H-3a,7-Methanoazulene, octahydro-1,9,9-trimethyl-	204	C15H24	000508-55-4	53
4	1,4-Dimethyl-8-isopropylidenetriazolo[4,5-b]pyridine	204	C15H24	1000140-07-7	52
5	Farnesyl bromide	284	C15H25Br	006874-67-5	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG021720\
Data File : BG044459.D
Acq On : 17 Feb 2020 22:55
Operator : CG/JU
Sample : L1547-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MARCY-GREEN-BH-03-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.99	2.2	ng	47706	1	7.89	431742	20.0
5-Eicosene, (E)-	21.18	5.4	ng	379172	5	21.51	1405610	20.0
Ethanol, 2-(dodec...	22.31	3.0	ng	209335	5	21.51	1405610	20.0
Tetracosane	23.73	2.3	ng	168205	6	24.59	1488120	20.0
Hexacosane	25.71	2.9	ng	217077	6	24.59	1488120	20.0
1,2,4,8-Tetrameth...	28.58	6.9	ng	515670	6	24.59	1488120	20.0