

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052620\
 Data File : BG045470.D
 Acq On : 26 May 2020 23:40
 Operator : CG/JU
 Sample : L2745-09
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 NM63-COMP-2020-0-6

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-BG051520.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	3.117	3	5	23	rVB	153665	234892	6.36%	0.957%
2	5.561	414	421	432	rBV	710591	1247981	33.77%	5.087%
3	7.177	689	696	707	rBV	804711	1490465	40.33%	6.075%
4	7.964	822	830	838	rBV	299042	519431	14.06%	2.117%
5	8.287	875	885	895	rBV	771148	1367692	37.01%	5.575%
6	9.121	1019	1027	1038	rBV	568854	1085340	29.37%	4.424%
7	10.772	1300	1308	1317	rBV	392905	740059	20.03%	3.016%
8	13.227	1717	1726	1735	rBV	1706535	2725790	73.76%	11.110%
9	14.056	1860	1867	1878	rBV	185996	281219	7.61%	1.146%
10	14.602	1953	1960	1967	rBV	627000	1047790	28.35%	4.271%
11	16.100	2208	2215	2226	rBV	1338956	2037774	55.14%	8.306%
12	17.351	2418	2428	2433	rBV	794824	1246524	33.73%	5.081%
13	17.392	2433	2435	2442	rVB2	63182	87837	2.38%	0.358%
14	18.256	2579	2582	2589	rVB5	20003	42786	1.16%	0.174%
15	19.407	2772	2778	2784	rVB	201867	297620	8.05%	1.213%
16	19.765	2829	2839	2846	rBV	204986	387739	10.49%	1.580%
17	19.965	2867	2873	2881	rBV	2813601	3695417	100.00%	15.062%
18	20.094	2889	2895	2896	rBV5	26862	47301	1.28%	0.193%
19	20.359	2936	2940	2946	rBV6	29190	55515	1.50%	0.226%
20	20.418	2947	2950	2954	rVB	35074	46258	1.25%	0.189%
21	20.770	3005	3010	3013	rBV6	36869	47985	1.30%	0.196%
22	20.823	3015	3019	3023	rBV7	26977	43490	1.18%	0.177%
23	21.269	3091	3095	3103	rVB4	141387	235959	6.39%	0.962%
24	21.610	3145	3153	3158	rBV3	798763	1522911	41.21%	6.207%
25	21.810	3183	3187	3192	rVB4	82464	122814	3.32%	0.501%
26	21.951	3207	3211	3215	rVB7	76951	122269	3.31%	0.498%
27	22.409	3285	3289	3298	rVB2	107875	186881	5.06%	0.762%
28	23.090	3399	3405	3412	rVB	121272	226675	6.13%	0.924%
29	23.760	3513	3519	3529	rBV2	91815	332678	9.00%	1.356%
30	23.878	3534	3539	3546	rVB3	108339	238580	6.46%	0.972%
31	24.471	3633	3640	3650	rVB	64519	203466	5.51%	0.829%
32	24.606	3658	3663	3676	rVB	75536	207370	5.61%	0.845%
33	24.765	3680	3690	3708	rVB2	463909	1588322	42.98%	6.474%
34	25.904	3880	3884	3896	rVB5	83359	234389	6.34%	0.955%

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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 >
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35	27.226	4105	4109	4122	rVB5	38781	118567	3.21%	0.483%
36	28.330	4291	4297	4299	rBV4	22349	49028	1.33%	0.200%
37	28.859	4378	4387	4398	rVB4	97248	367351	9.94%	1.497%

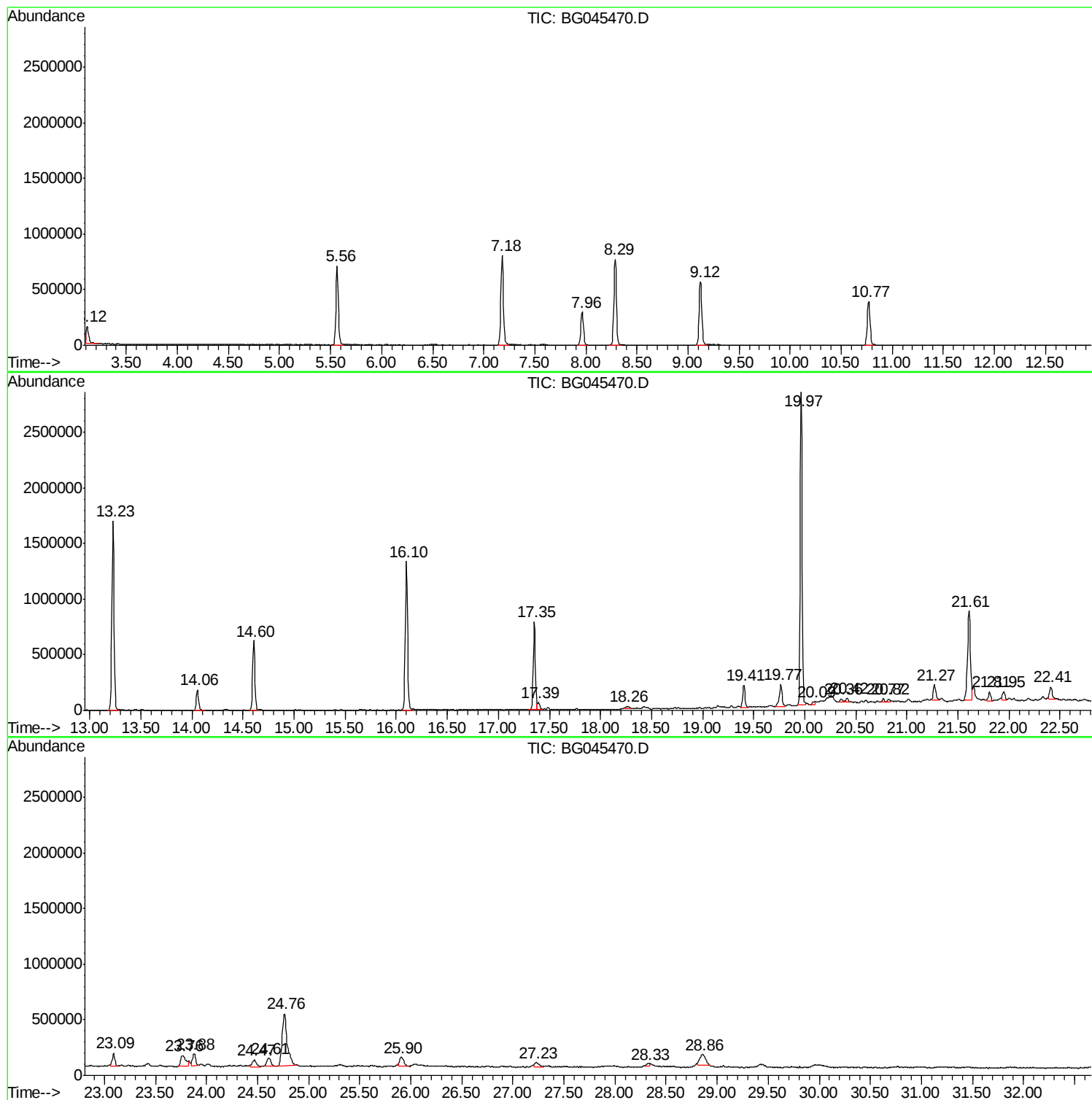
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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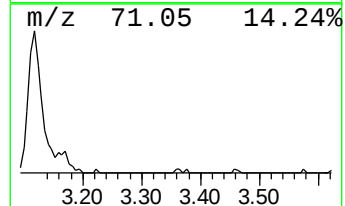
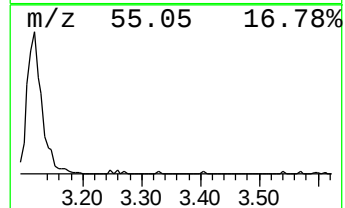
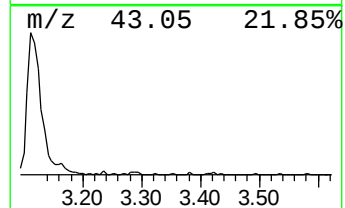
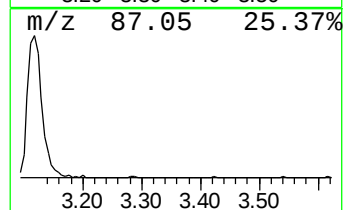
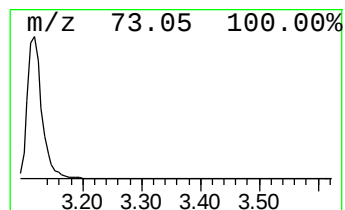
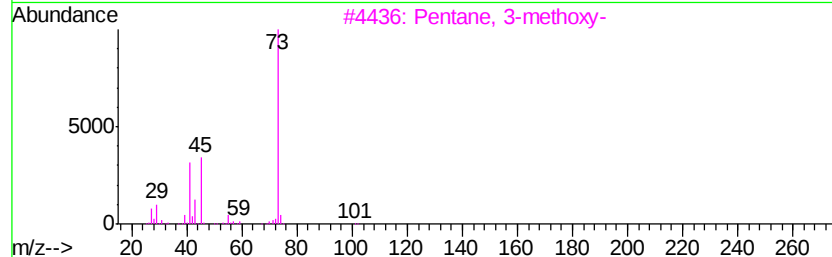
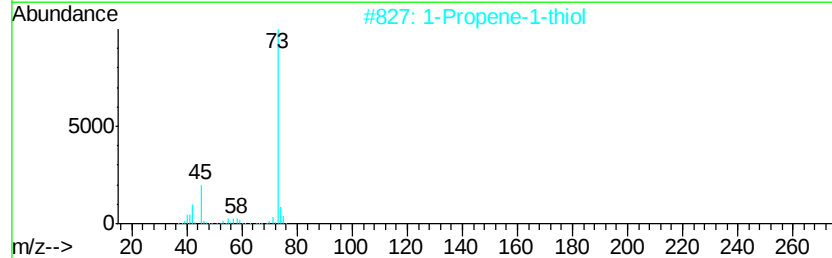
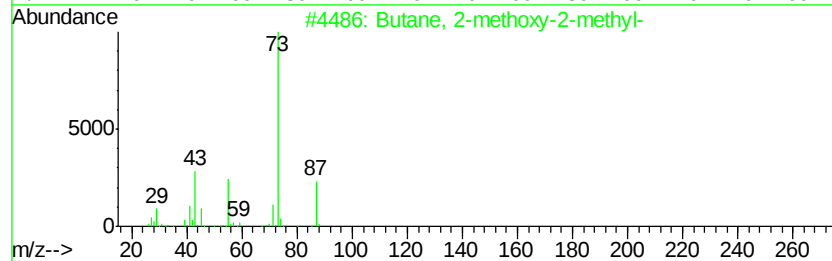
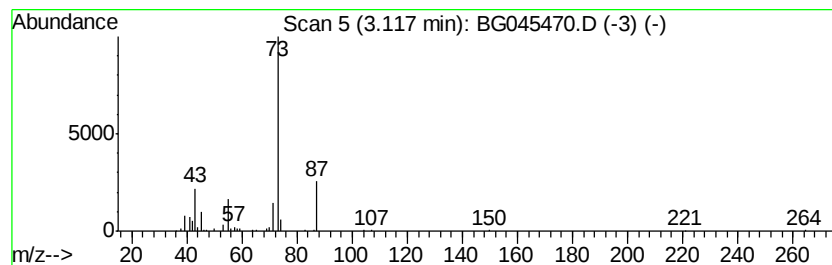
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	9.04 ng	234892	1,4-Dichlorobenzene-d4	7.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			1-Propene-1-thiol	74	C3H6S	000925-89-3	16
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4			2-(2-Bromoethyl)-1,3-dioxolane	180	C5H9BrO2	018742-02-4	9
5			1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9



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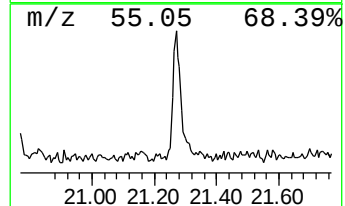
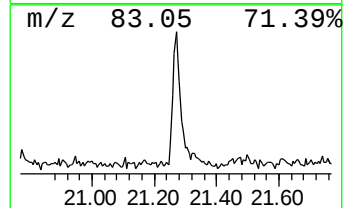
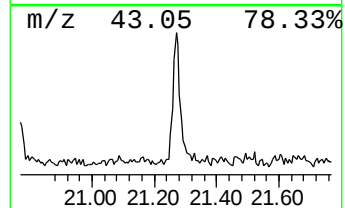
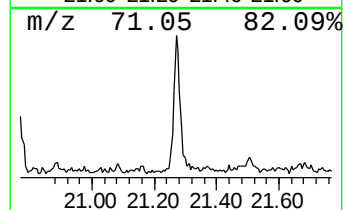
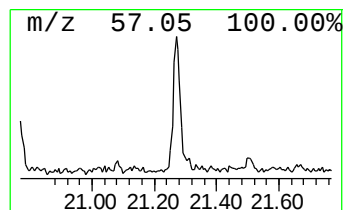
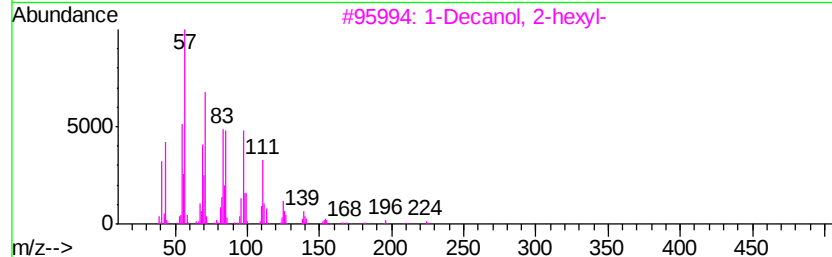
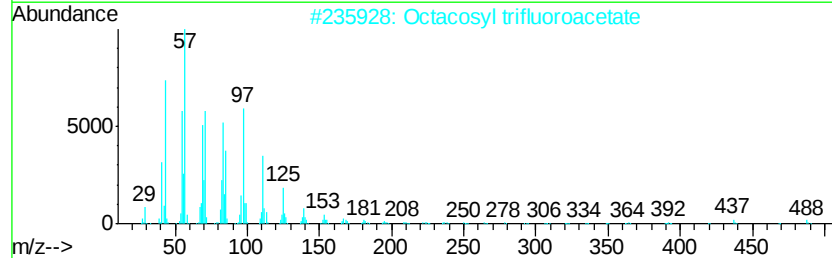
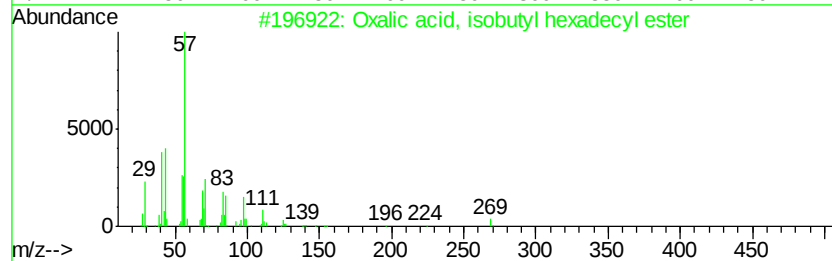
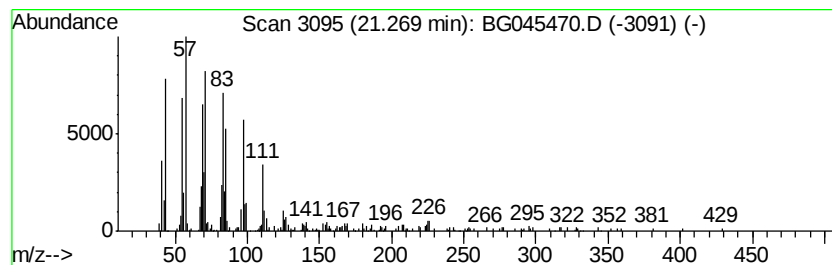
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Peak Number 3 Oxalic acid, isobutyl hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.27	3.10 ng	235959	Chrysene-d12	21.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
3		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
4		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
5		Hexadecane	226	C16H34	000544-76-3	90



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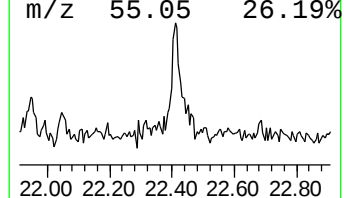
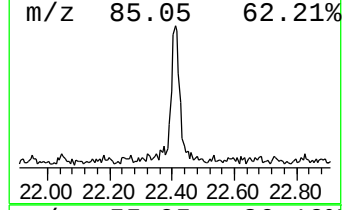
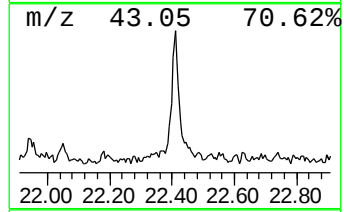
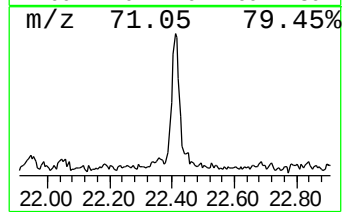
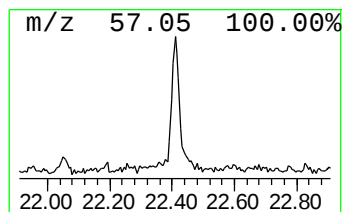
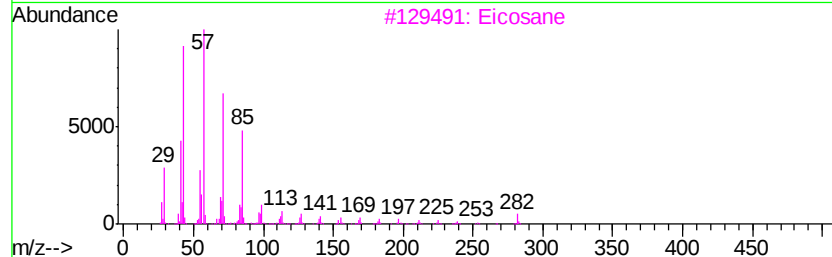
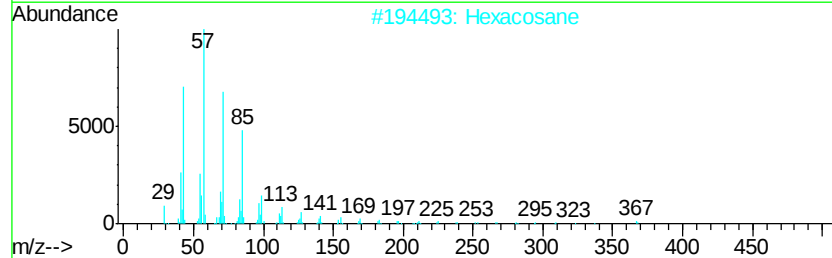
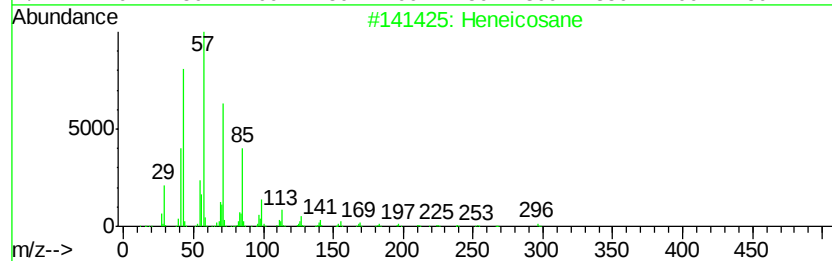
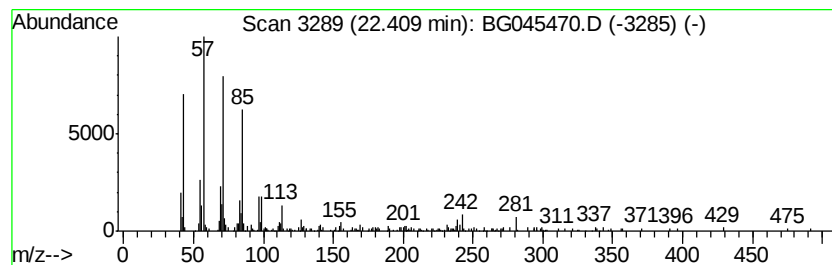
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Peak Number 4 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	2.45 ng	186881	Chrysene-d12	21.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	89
2		Hexacosane	366	C26H54	000630-01-3	87
3		Eicosane	282	C20H42	000112-95-8	86
4		Tetradecane, 6,9-dimethyl-	226	C16H34	055045-13-1	83
5		Hexadecane	226	C16H34	000544-76-3	83



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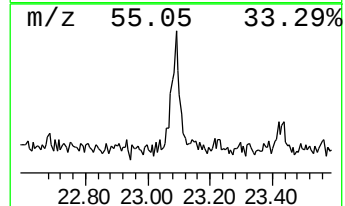
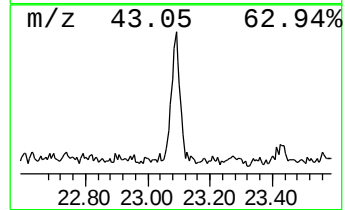
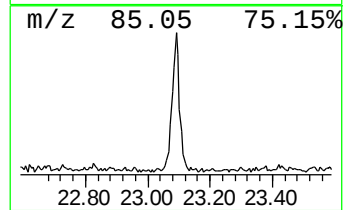
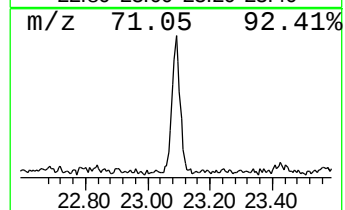
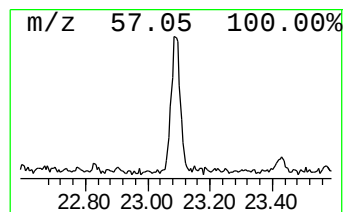
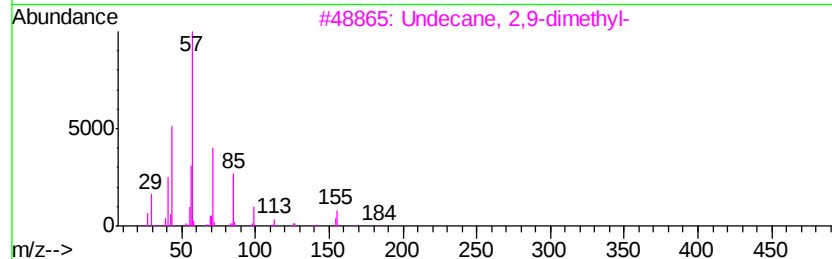
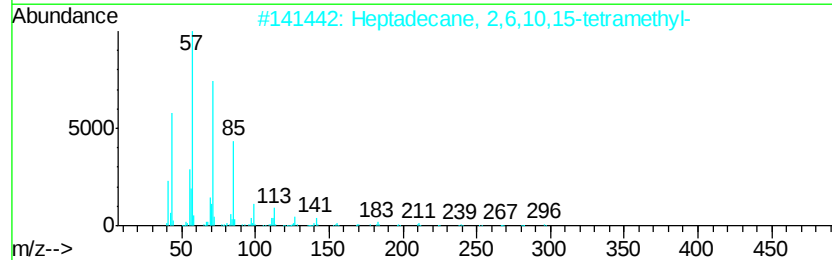
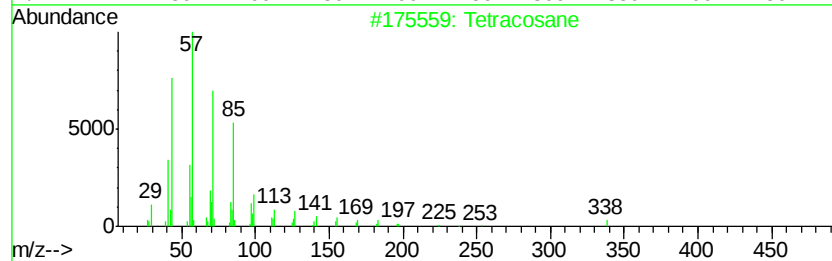
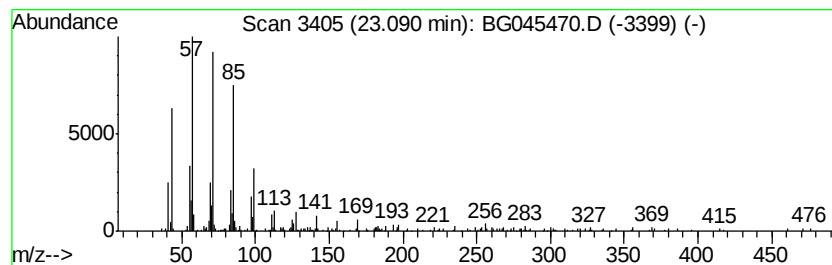
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.09	2.98 ng	226675	Chrysene-d12	21.61

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	90
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
3		Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	86
4		2-methyloctacosane	408	C29H60	1000376-72-8	86
5		Heneicosane	296	C21H44	000629-94-7	86



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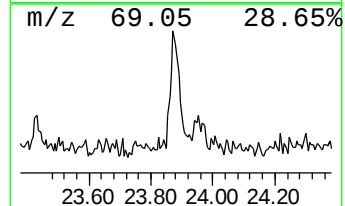
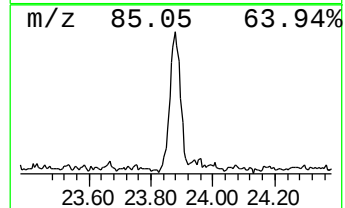
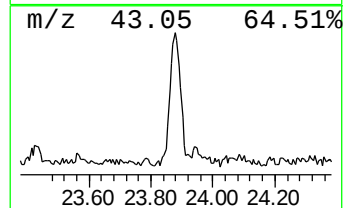
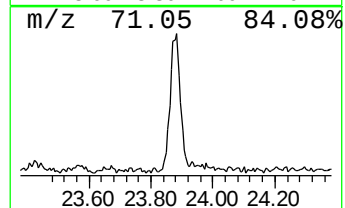
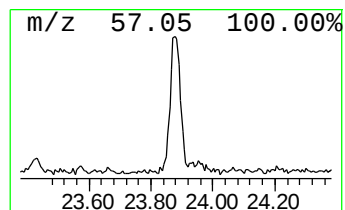
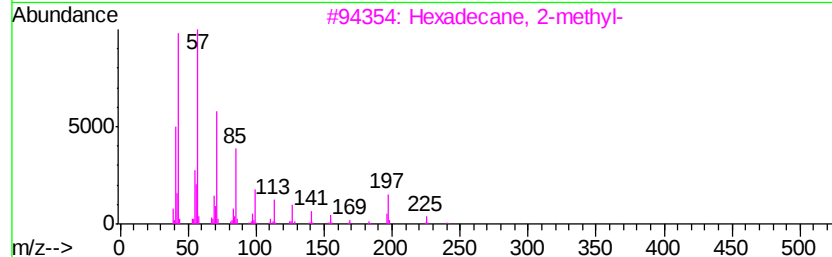
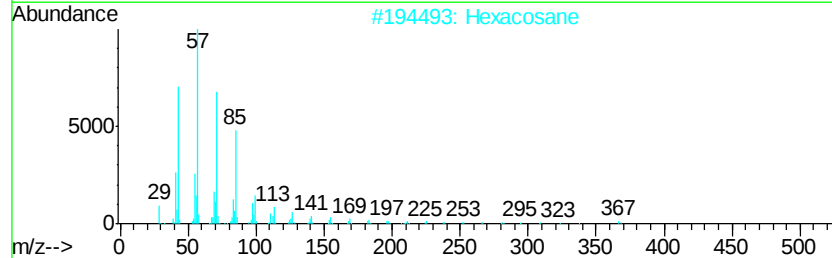
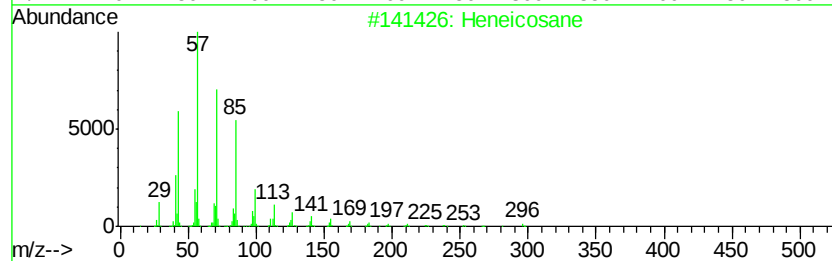
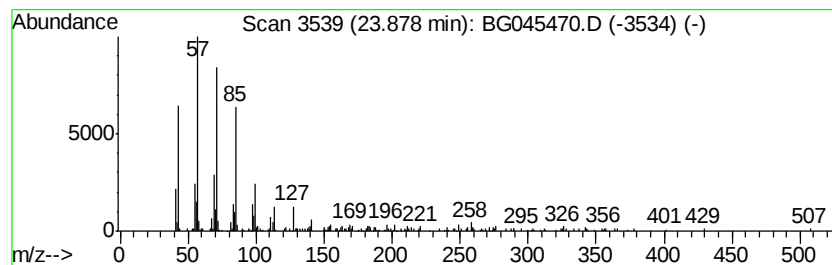
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Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.88	3.00 ng	238580	Perylene-d12	24.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Hexacosane	366	C26H54	000630-01-3	87
3		Hexadecane, 2-methyl-	240	C17H36	001560-92-5	86
4		2-methyloctacosane	408	C29H60	1000376-72-8	86
5		Tetracosane	338	C24H50	000646-31-1	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052620\
Data File : BG045470.D
Acq On : 26 May 2020 23:40
Operator : CG/JU
Sample : L2745-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NM63-COMP-2020-0-6

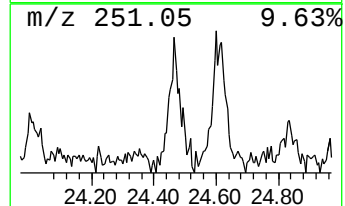
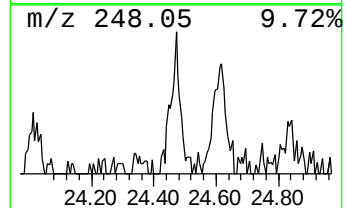
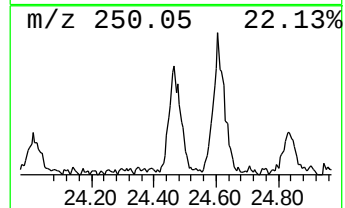
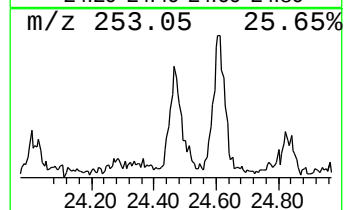
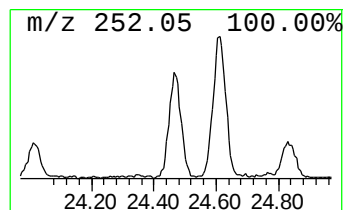
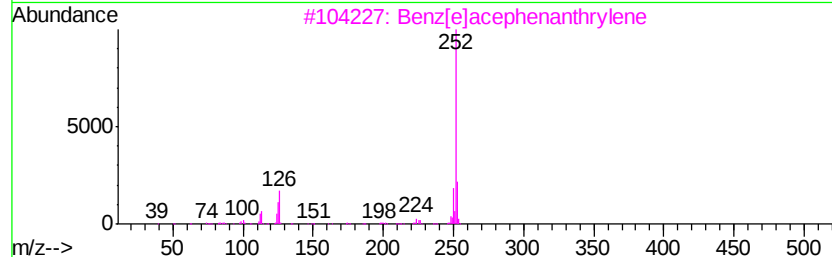
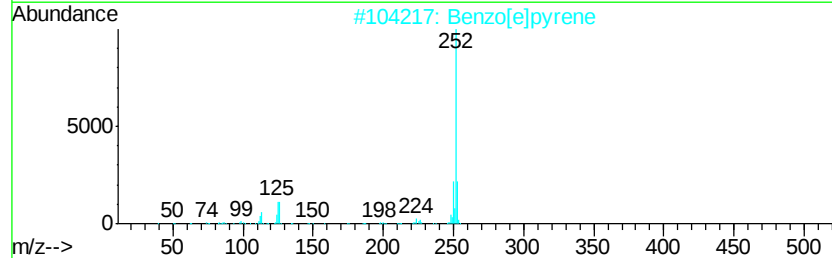
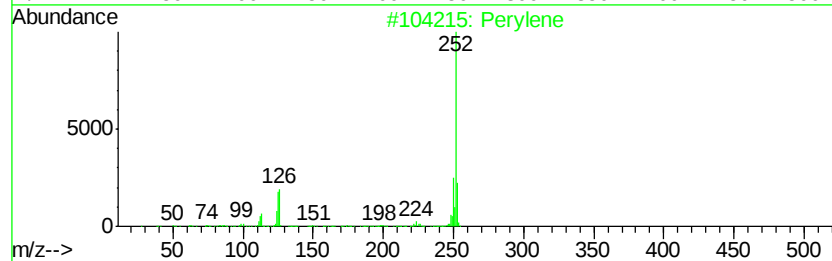
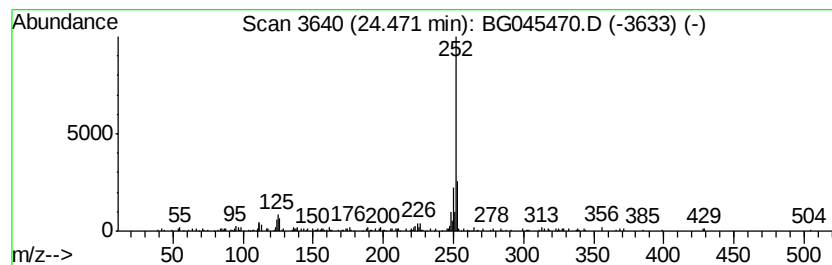
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Perylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.47	2.56 ng	203466	Perylene-d12	24.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene		252	C20H12	000198-55-0	89
2	Benzo[e]pyrene		252	C20H12	000192-97-2	81
3	Benz[e]acephenanthrylene		252	C20H12	000205-99-2	74
4	(1-Cyclopentenyl)ferrocene		252	C15H16Fe	012260-67-2	72
5	Benzo[a]pyrene		252	C20H12	000050-32-8	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052620\
Data File : BG045470.D
Acq On : 26 May 2020 23:40
Operator : CG/JU
Sample : L2745-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NM63-COMP-2020-0-6

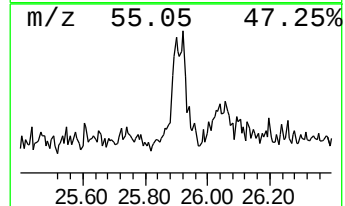
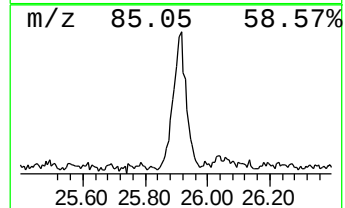
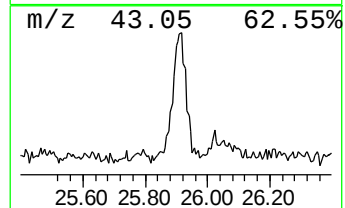
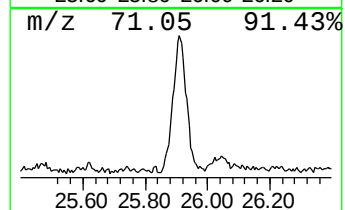
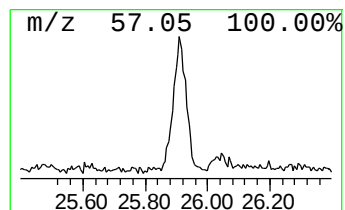
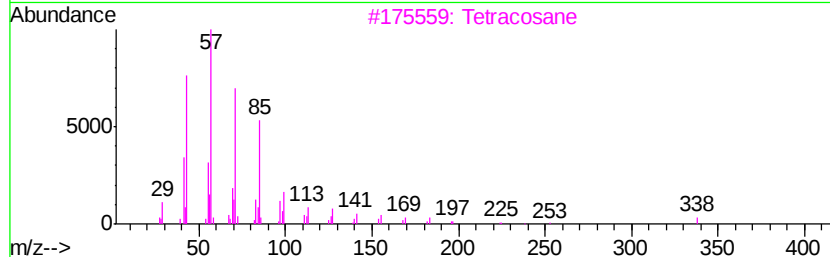
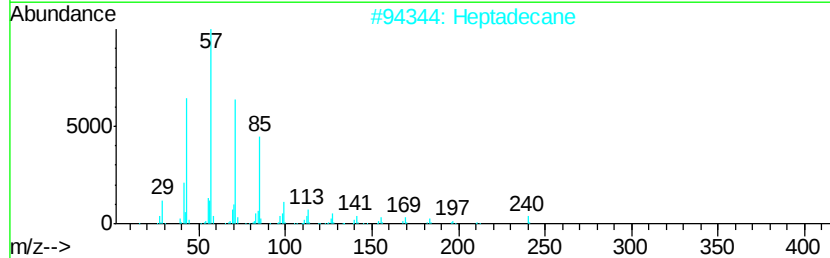
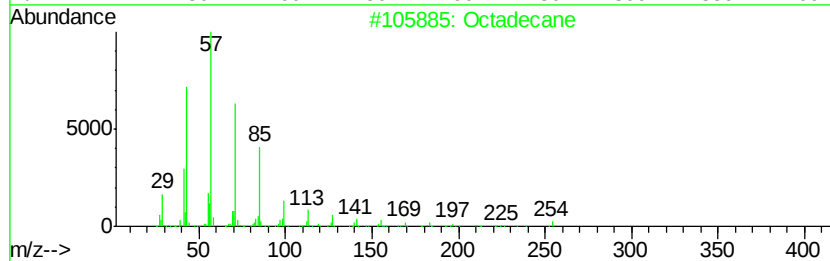
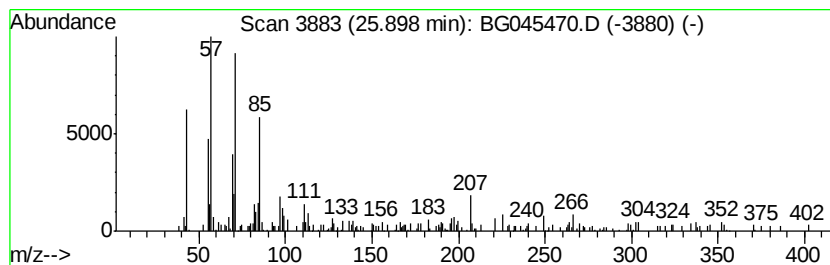
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.90	2.95 ng	234389	Perylene-d12	24.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	86
2	Heptadecane		240	C17H36	000629-78-7	83
3	Tetracosane		338	C24H50	000646-31-1	78
4	Heptacosane		380	C27H56	000593-49-7	74
5	Nonane, 1-iodo-		254	C9H19I	004282-42-2	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052620\
Data File : BG045470.D
Acq On : 26 May 2020 23:40
Operator : CG/JU
Sample : L2745-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

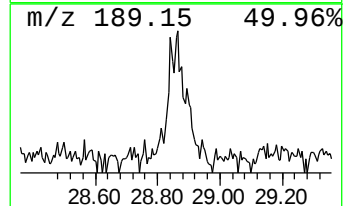
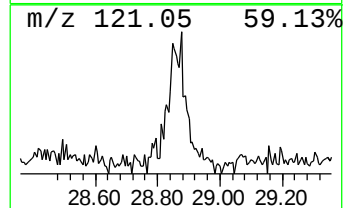
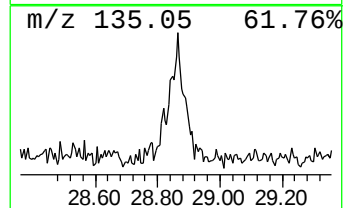
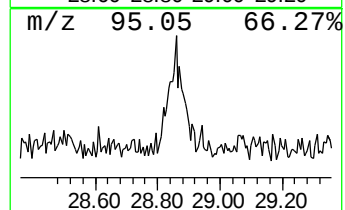
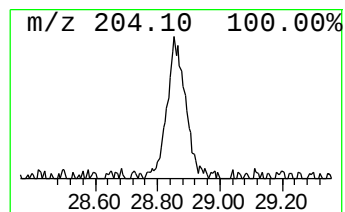
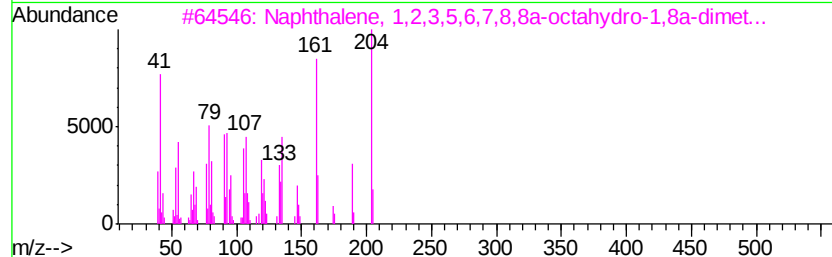
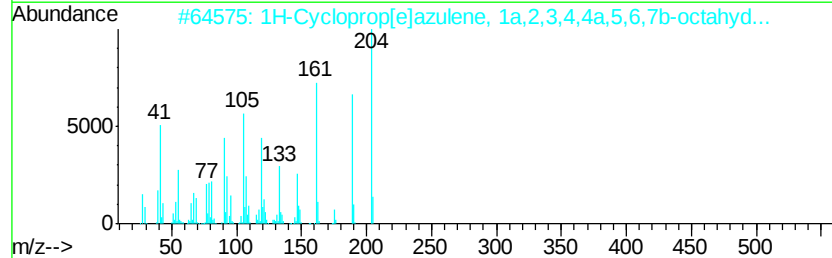
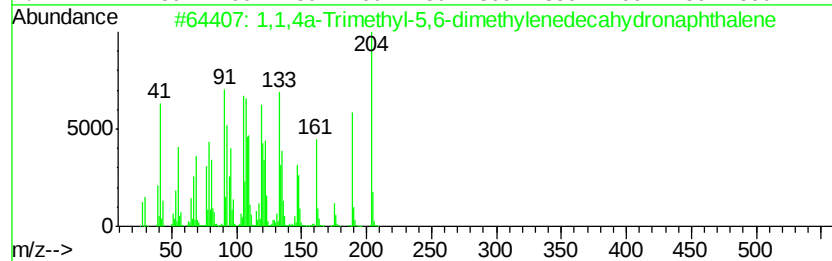
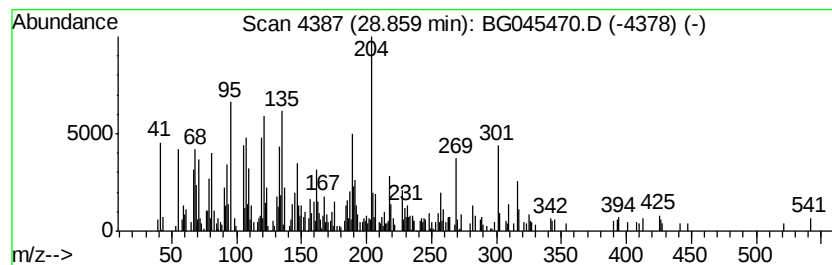
Instrument :
BNA_G
ClientSampleId :
NM63-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.86	4.63 ng	367351	Perylene-d12	24.76
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204 C15H24	1000193-60-8	83
2	1H-Cycloprop[e]azulene, 1a,2,3,4...	204 C15H24	000489-40-7	64
3	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204 C15H24	004630-07-3	64
4	1H-3a,7-Methanoazulene, 2,3,6,7,...	204 C15H24	000560-32-7	55
5	Guaia-3,9-diene	204 C15H24	000489-83-8	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052620\
Data File : BG045470.D
Acq On : 26 May 2020 23:40
Operator : CG/JU
Sample : L2745-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NM63-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.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
Butane, 2-methoxy...	3.12	9.0	ng	234892	1	7.96	519431	20.0
Oxalic acid, isob...	21.27	3.1	ng	235959	5	21.61	1522910	20.0
Heneicosane	22.41	2.5	ng	186881	5	21.61	1522910	20.0
Tetracosane	23.09	3.0	ng	226675	5	21.61	1522910	20.0
Hexacosane	23.88	3.0	ng	238580	6	24.76	1588320	20.0
Perylene	24.47	2.6	ng	203466	6	24.76	1588320	20.0
Octadecane	25.90	3.0	ng	234389	6	24.76	1588320	20.0
1,1,4a-Trimethyl-...	28.86	4.6	ng	367351	6	24.76	1588320	20.0