

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061523\
 Data File : BG057732.D
 Acq On : 15 Jun 2023 20:16
 Operator : CG/JU
 Sample : 03222-01 2X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMP-SB-33

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057732.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.139	3	9	20	rVB4	48921	123817	11.30%	0.981%
2	5.049	328	334	343	rVB	29628	48727	4.45%	0.386%
3	5.513	406	413	422	rBV	331800	564707	51.53%	4.473%
4	7.088	674	681	690	rBV	348472	594454	54.25%	4.708%
5	7.934	818	825	834	rBV	154286	261006	23.82%	2.067%
6	9.091	1015	1022	1030	rBV	191795	337623	30.81%	2.674%
7	10.736	1293	1302	1308	rBV	207287	373814	34.11%	2.961%
8	13.192	1713	1720	1727	rBV	512115	763404	69.66%	6.047%
9	14.567	1946	1954	1960	rBV	294500	458231	41.81%	3.629%
10	14.626	1960	1964	1970	rVB	12859	19420	1.77%	0.154%
11	14.961	2016	2021	2025	rVB	10637	14329	1.31%	0.113%
12	15.613	2127	2132	2140	rBV	16817	24607	2.25%	0.195%
13	15.919	2177	2184	2190	rVB	90605	134187	12.24%	1.063%
14	16.048	2198	2206	2217	rBV	356742	544721	49.71%	4.315%
15	16.277	2242	2245	2254	rBV4	9202	18330	1.67%	0.145%
16	16.959	2357	2361	2367	rVB3	8539	13442	1.23%	0.106%
17	17.123	2385	2389	2396	rVB2	10088	15910	1.45%	0.126%
18	17.311	2414	2421	2425	rBV	366695	571570	52.16%	4.527%
19	17.352	2425	2428	2434	rVV	185729	255585	23.32%	2.024%
20	17.440	2438	2443	2448	rVV	45086	67062	6.12%	0.531%
21	17.705	2480	2488	2493	rBV2	17455	34072	3.11%	0.270%
22	18.187	2565	2570	2574	rBV	33328	54259	4.95%	0.430%
23	18.234	2574	2578	2584	rVV	40921	66954	6.11%	0.530%
24	18.310	2587	2591	2596	rVV	15872	25180	2.30%	0.199%
25	18.380	2596	2603	2607	rVV3	47550	94708	8.64%	0.750%
26	18.416	2607	2609	2614	rVB	21582	27451	2.50%	0.217%
27	18.686	2649	2655	2658	rBV	26138	42088	3.84%	0.333%
28	18.721	2658	2661	2667	rVB4	17202	26332	2.40%	0.209%
29	18.927	2693	2696	2701	rBV6	8418	11941	1.09%	0.095%
30	18.980	2701	2705	2708	rVV	8819	13555	1.24%	0.107%
31	19.021	2708	2712	2716	rVB4	9749	12484	1.14%	0.099%
32	19.097	2721	2725	2728	rBV2	24019	37571	3.43%	0.298%
33	19.238	2745	2749	2756	rVB3	21182	32403	2.96%	0.257%
34	19.362	2764	2770	2778	rBV	411053	565351	51.59%	4.478%
35	19.426	2778	2781	2783	rBV2	9394	11192	1.02%	0.089%
36	19.456	2783	2786	2791	rVB5	10232	14546	1.33%	0.115%

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Min Area: 3 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	19.726	2820	2832	2839	rBV	361559	654523	59.73%	5.184%
38	19.791	2840	2843	2851	rVB3	20451	35842	3.27%	0.284%
39	19.926	2858	2866	2871	rBV	828444	1095859	100.00%	8.680%
40	20.043	2881	2886	2893	rBV4	31752	79163	7.22%	0.627%
41	20.184	2905	2910	2911	rBV4	21358	30685	2.80%	0.243%
42	20.214	2911	2915	2922	rVB2	58136	96285	8.79%	0.763%
43	20.313	2928	2932	2936	rBV2	40942	57450	5.24%	0.455%
44	20.372	2937	2942	2946	rVV2	41621	65666	5.99%	0.520%
45	20.413	2946	2949	2952	rVB3	14856	18228	1.66%	0.144%
46	20.513	2963	2966	2969	rBV	27351	32427	2.96%	0.257%
47	20.560	2969	2974	2978	rVB3	25608	38301	3.50%	0.303%
48	20.666	2990	2992	2997	rVB6	21674	22885	2.09%	0.181%
49	20.731	3001	3003	3007	rVB2	12792	13016	1.19%	0.103%
50	20.966	3040	3043	3049	rVB2	34102	54048	4.93%	0.428%
51	21.154	3073	3075	3078	rVB	26174	24727	2.26%	0.196%
52	21.195	3079	3082	3084	rVV	25825	37355	3.41%	0.296%
53	21.230	3084	3088	3095	rVV5	84694	172010	15.70%	1.362%
54	21.295	3095	3099	3108	rVB2	39869	75935	6.93%	0.601%
55	21.465	3125	3128	3132	rVB	65799	80931	7.39%	0.641%
56	21.565	3136	3145	3150	rVV3	408322	1014679	92.59%	8.037%
57	21.612	3150	3153	3163	rVB	169742	273896	24.99%	2.169%
58	21.759	3174	3178	3184	rBV4	39076	75973	6.93%	0.602%
59	21.959	3208	3212	3219	rVB3	24678	47860	4.37%	0.379%
60	23.245	3426	3431	3439	rVB	64845	116327	10.62%	0.921%
61	23.727	3505	3513	3520	rBV	136798	454948	41.52%	3.603%
62	23.850	3529	3534	3539	rBV	62439	123686	11.29%	0.980%
63	24.426	3626	3632	3646	rVB2	89637	261273	23.84%	2.069%
64	24.573	3649	3657	3671	rVB2	117076	332554	30.35%	2.634%
65	24.726	3674	3683	3691	rBV	236502	643849	58.75%	5.100%
66	25.913	3878	3885	3893	rVB3	47826	132900	12.13%	1.053%
67	28.310	4285	4293	4307	rVB3	44016	186987	17.06%	1.481%

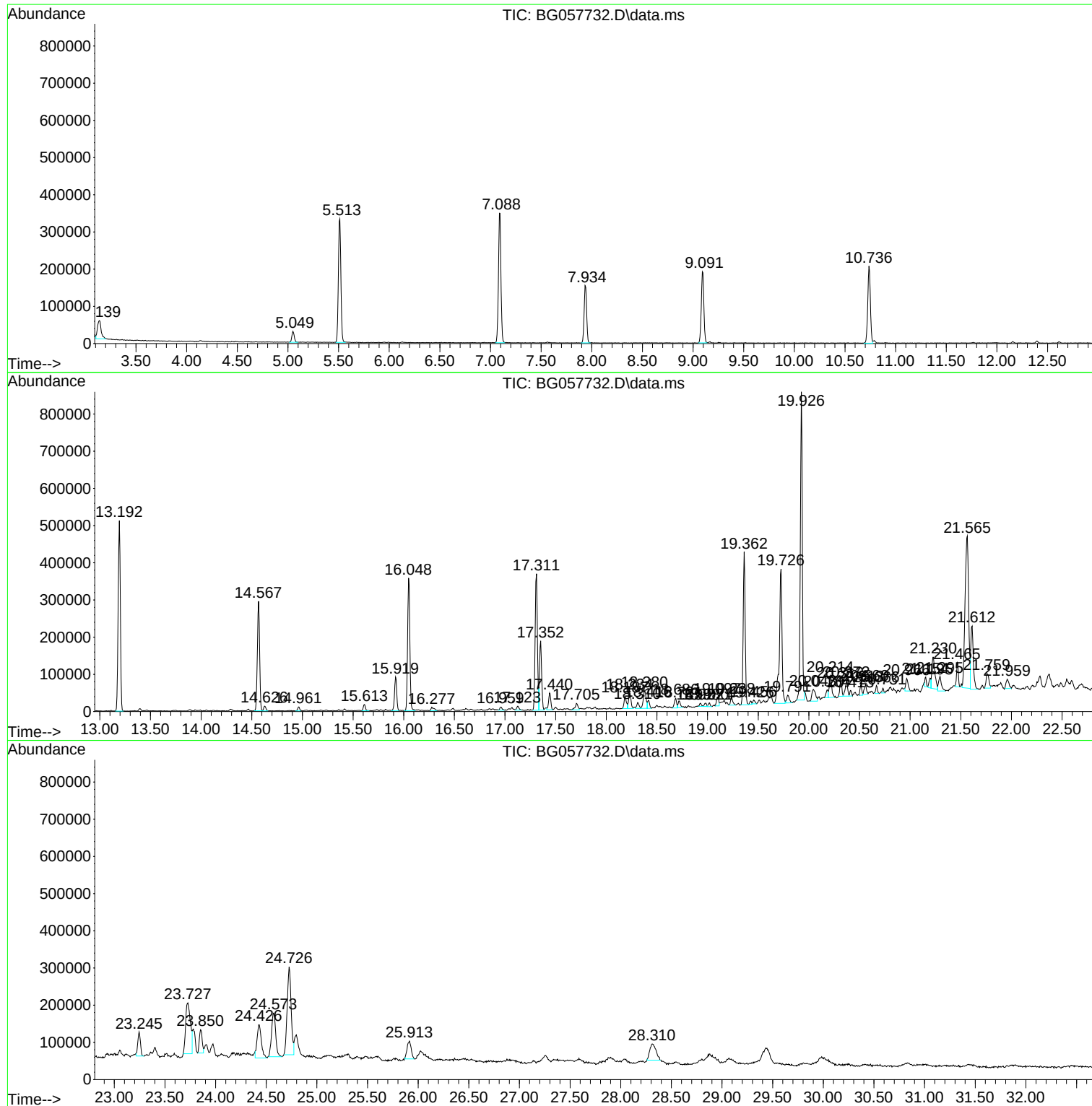
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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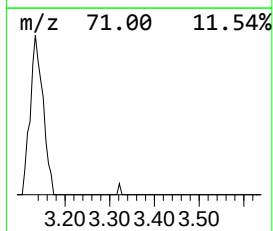
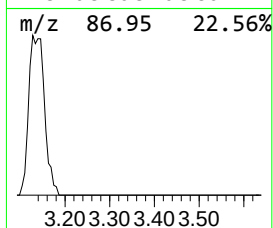
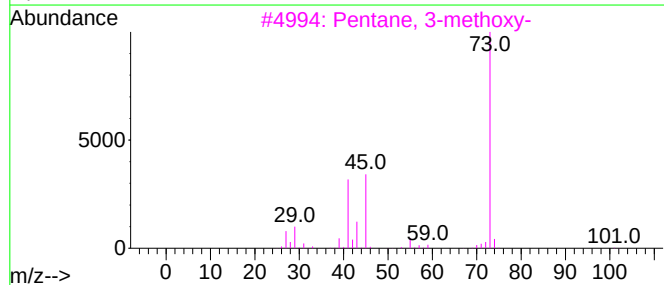
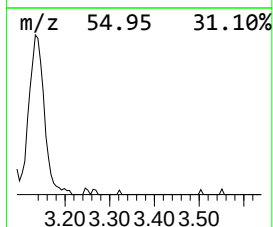
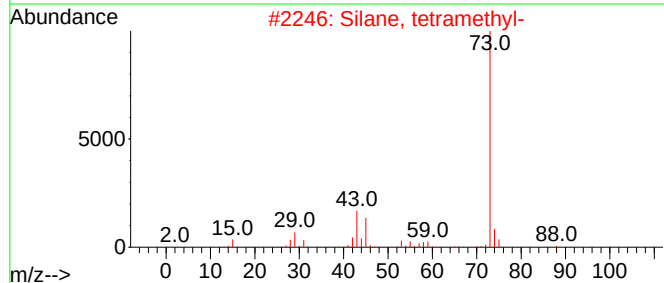
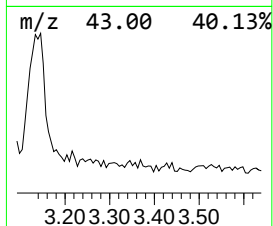
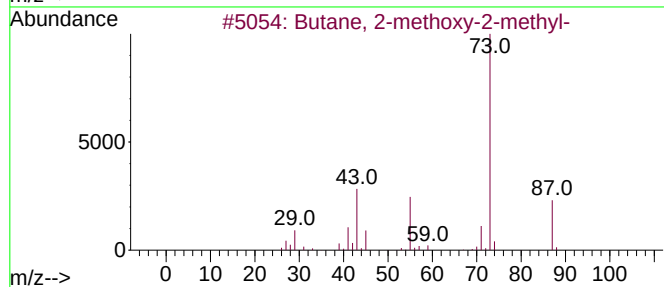
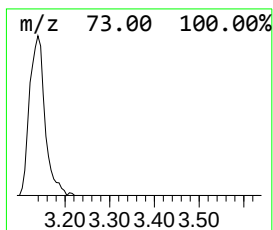
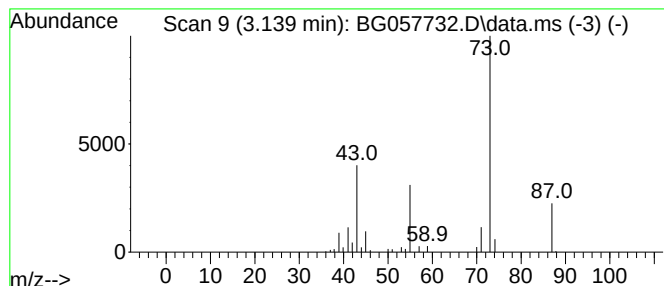
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.139	9.49 ng	123817	1,4-Dichlorobenzene-d4	7.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	27
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			1,4-Butanediamine	88	C4H12N2	000110-60-1	10
5			1-Propene-1-thiol	74	C3H6S	000925-89-3	9



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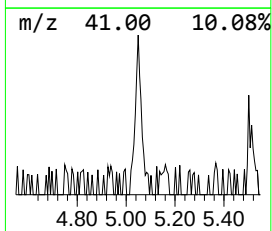
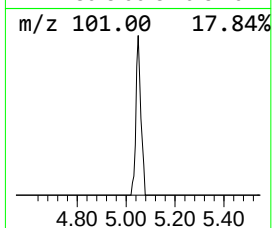
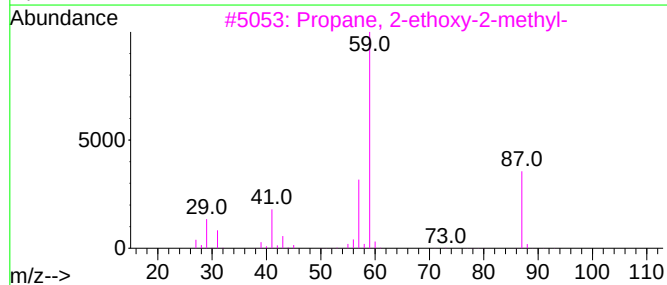
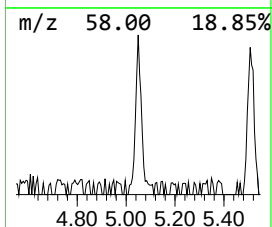
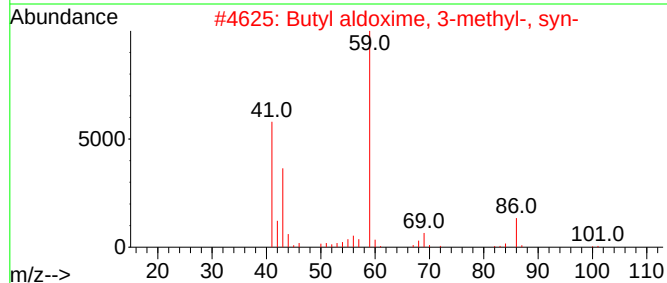
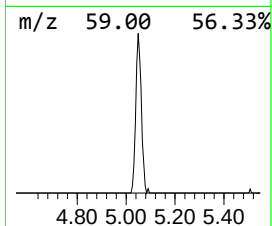
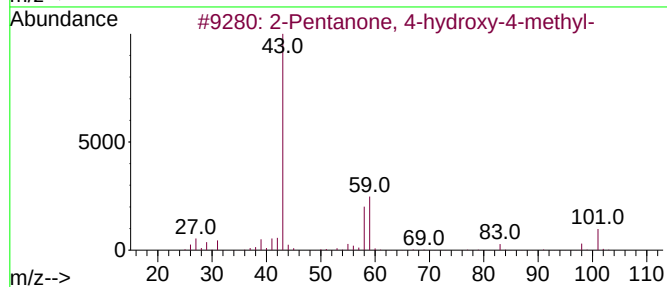
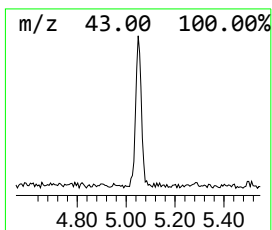
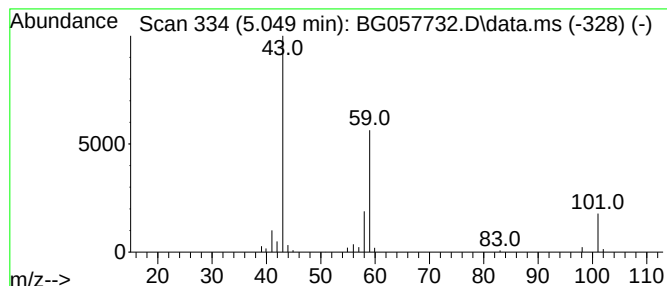
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.049	3.73 ng	48727	1,4-Dichlorobenzene-d4	7.934

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	37
3		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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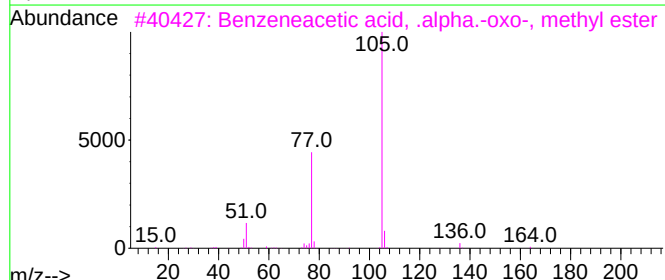
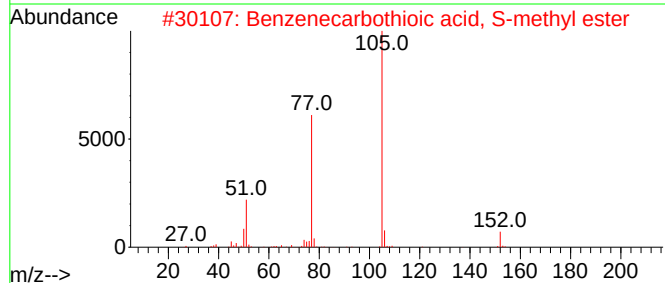
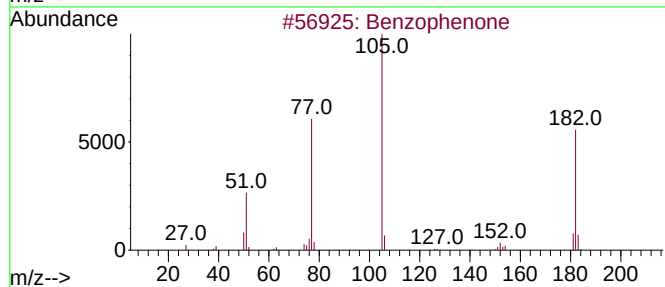
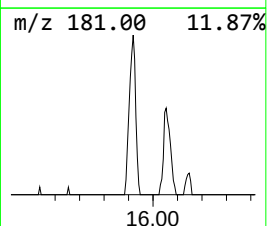
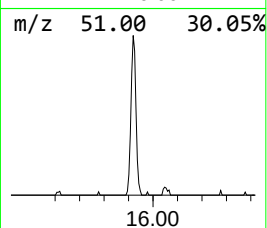
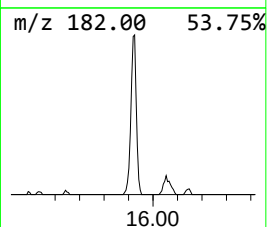
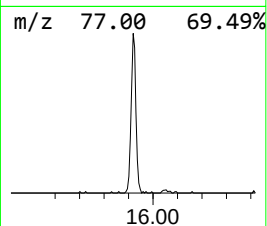
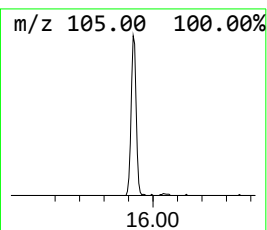
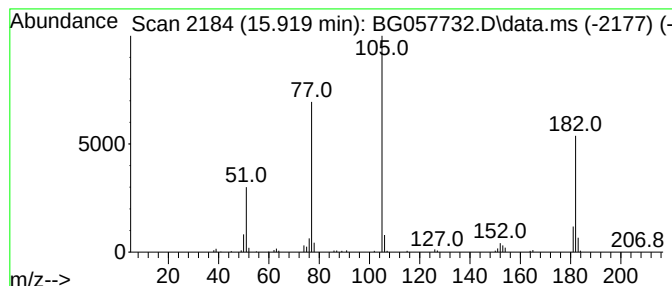
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.919	5.86 ng	134187	Acenaphthene-d10	14.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	53
3			Benzenecarbothioic acid, S-methyl ester	164	C9H8OS	015206-55-0	47
4			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47
5			Benzoyl bromide	184	C7H5BrO	000618-32-6	47



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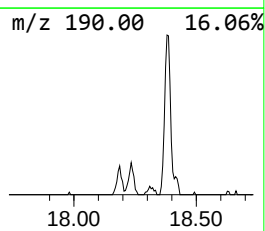
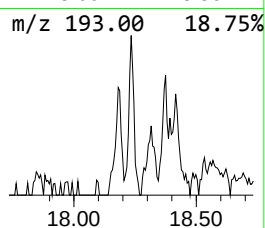
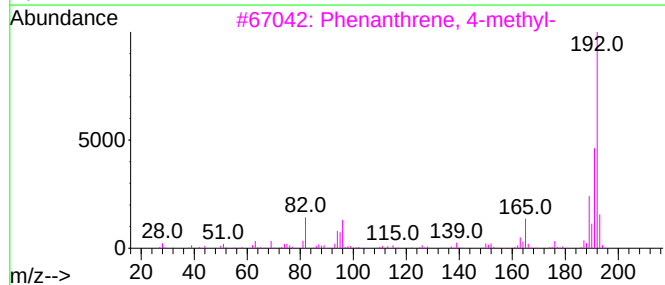
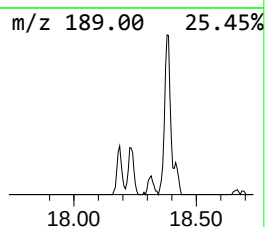
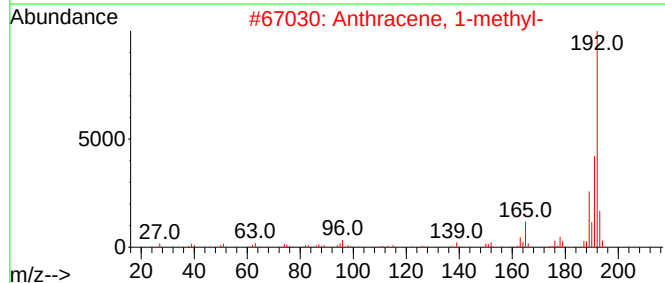
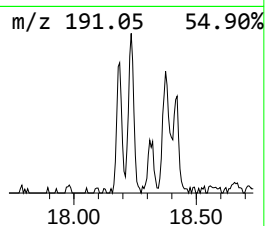
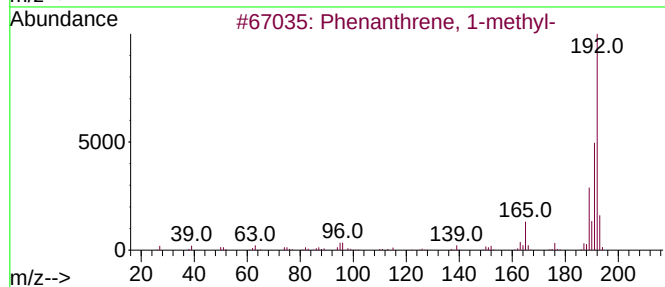
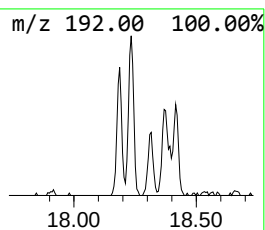
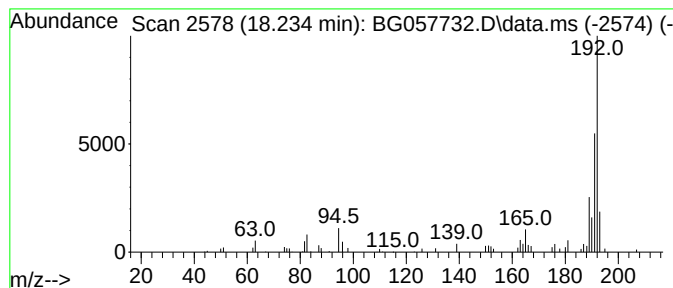
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	2.34 ng	66954	Phenanthrene-d10	17.311

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2			Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
3			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	90
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	90
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90



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ClientSampleId :
COMP-SB-33

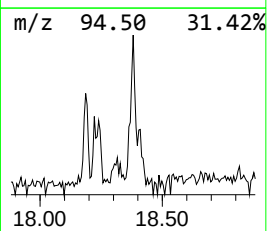
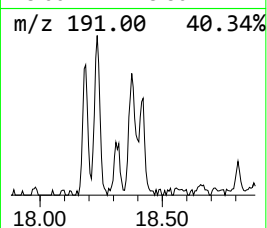
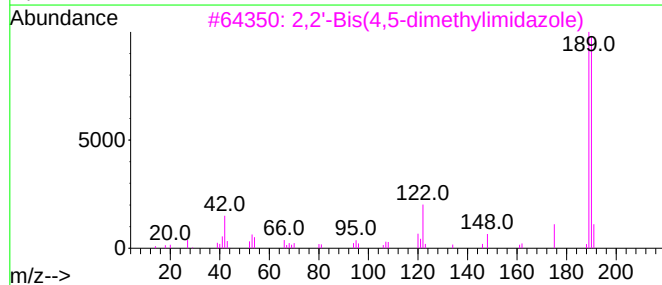
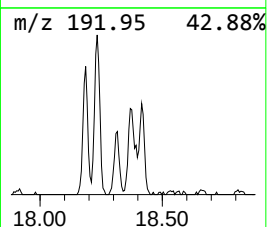
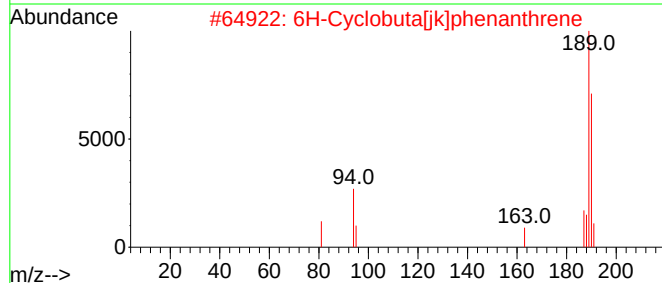
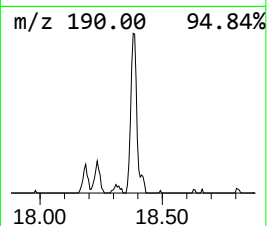
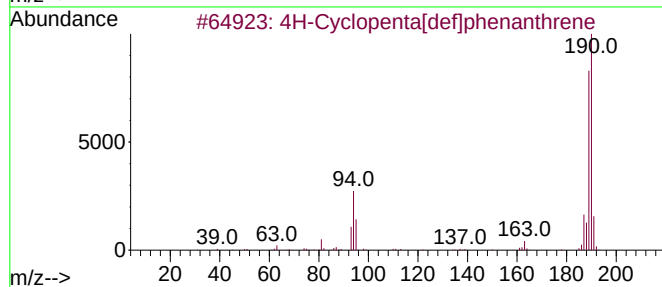
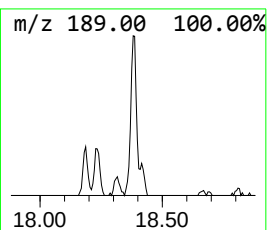
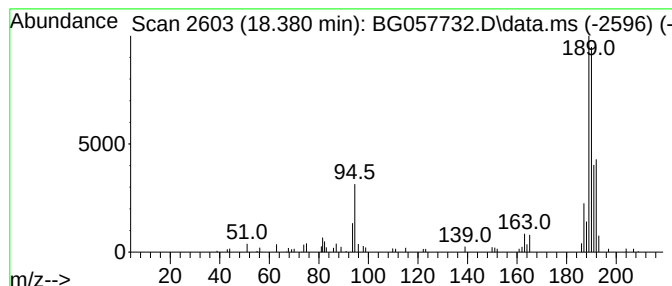
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.380	3.31 ng	94708	Phenanthrene-d10	17.311

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58
3			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	43
4			Methyl diselenide	190	C2H6Se2	007101-31-7	35
5			Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061523\
Data File : BG057732.D
Acq On : 15 Jun 2023 20:16
Operator : CG/JU
Sample : 03222-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-SB-33

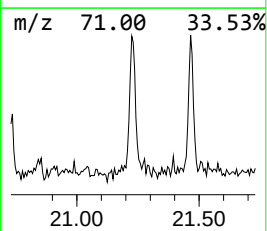
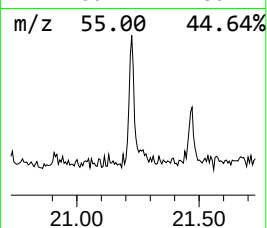
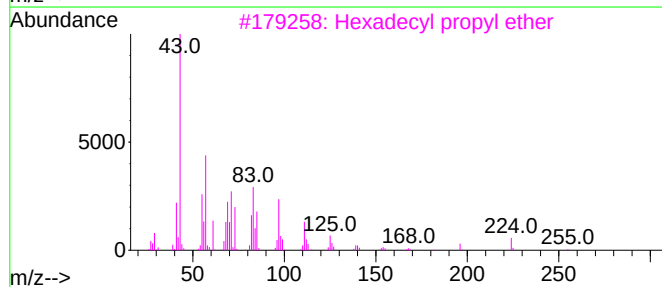
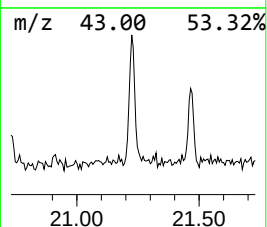
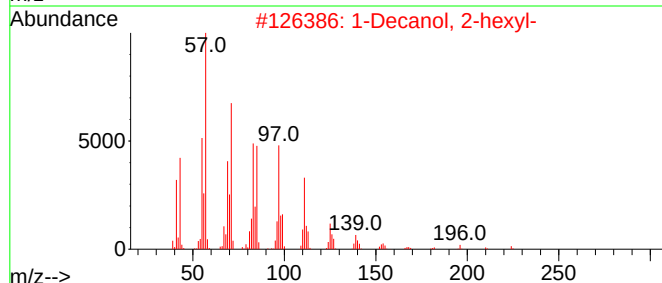
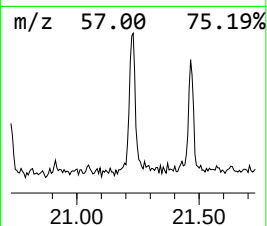
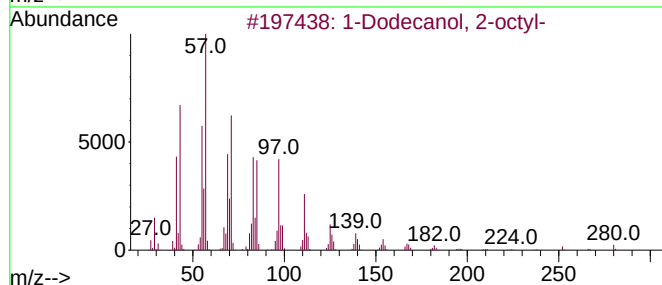
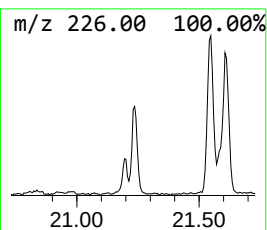
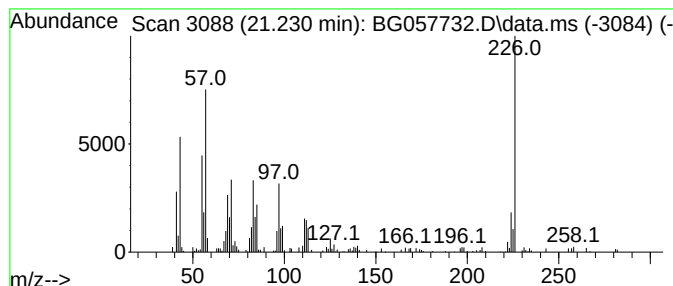
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown21.230 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.230	3.39 ng	172010	Chrysene-d12	21.565

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	30
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	25
3		Hexadecyl propyl ether	284	C19H40O	1000406-27-9	25
4		1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	25
5		1-Hexene-3,5-dione	112	C6H8O2	052204-69-0	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061523\
Data File : BG057732.D
Acq On : 15 Jun 2023 20:16
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Sample : 03222-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COMP-SB-33

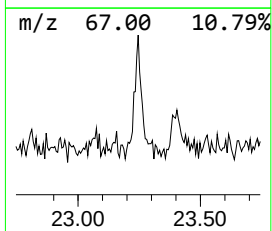
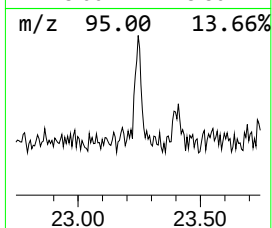
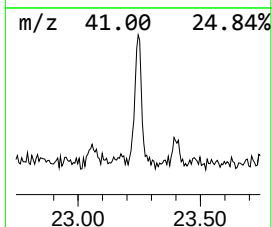
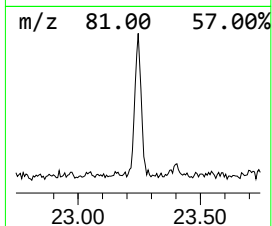
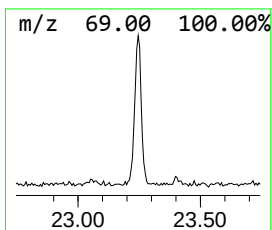
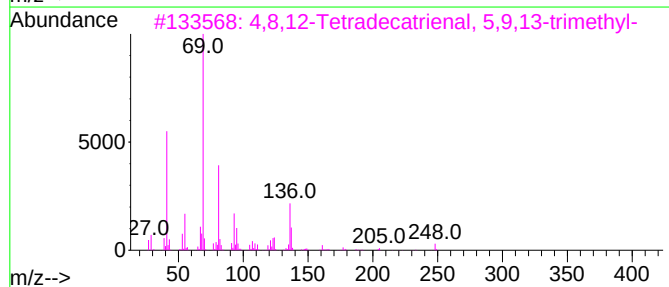
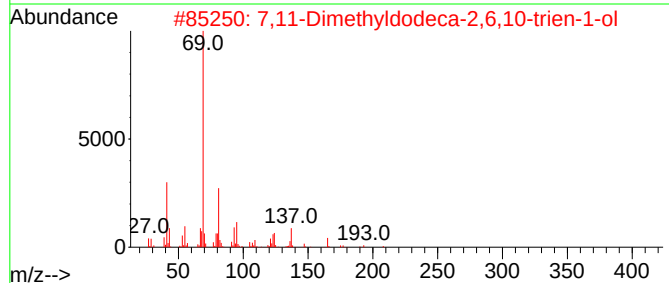
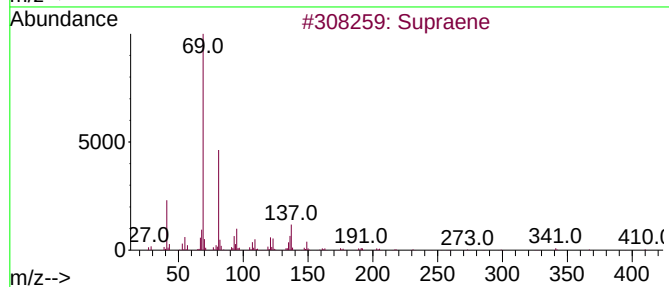
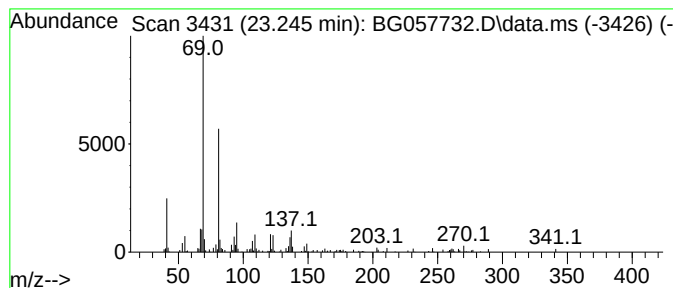
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.245	3.61 ng	116327	Perylene-d12	24.726

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	80
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	72
5			1,5-Heptadiene, 3,3,5-trimethyl-	138	C10H18	074630-29-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061523\
Data File : BG057732.D
Acq On : 15 Jun 2023 20:16
Operator : CG/JU
Sample : 03222-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COMP-SB-33

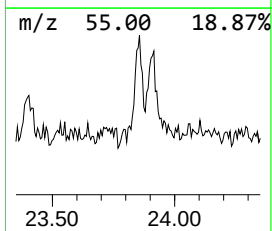
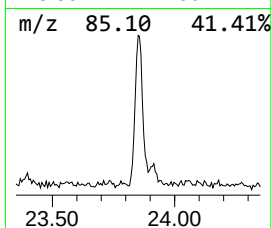
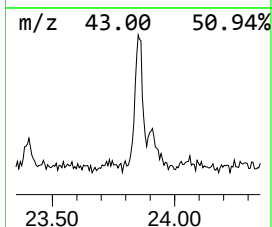
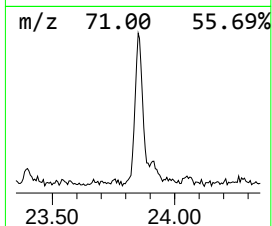
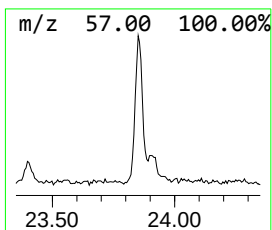
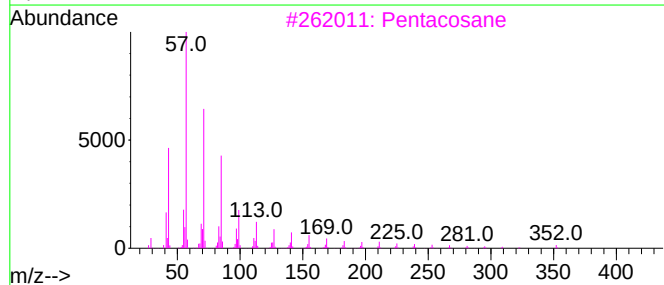
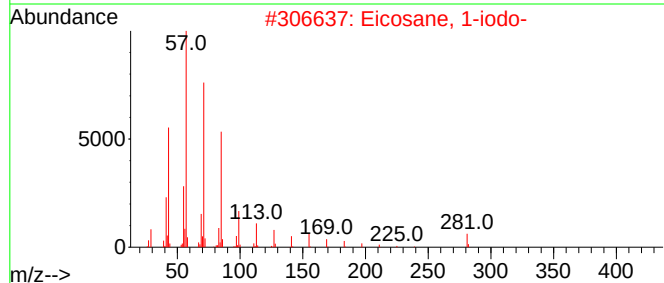
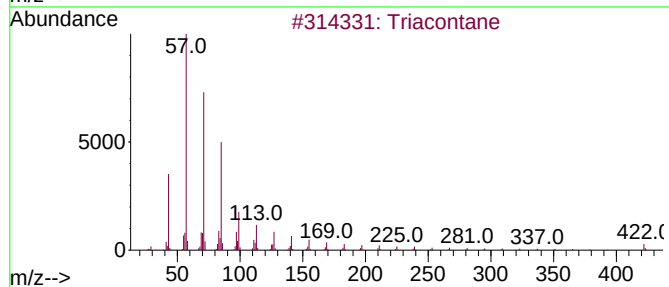
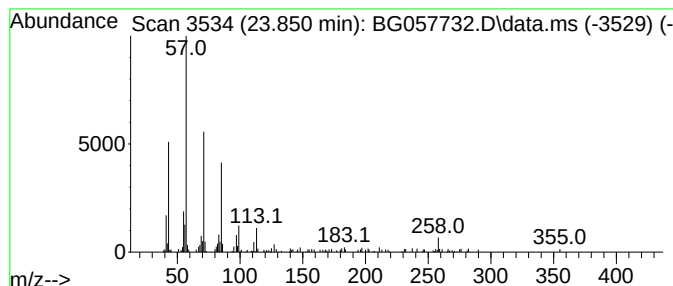
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.851	3.84 ng	123686	Perylene-d12	24.726

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	80
2			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	78
3			Pentacosane	352	C25H52	000629-99-2	72
4			Dodecane	170	C12H26	000112-40-3	72
5			Heptacosane	380	C27H56	000593-49-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061523\
Data File : BG057732.D
Acq On : 15 Jun 2023 20:16
Operator : CG/JU
Sample : 03222-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-SB-33

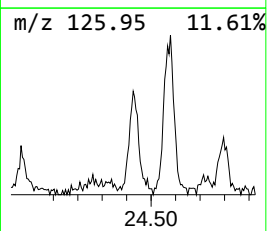
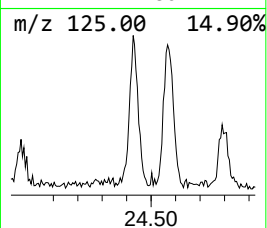
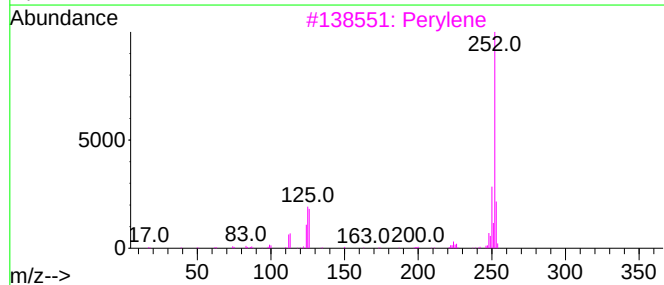
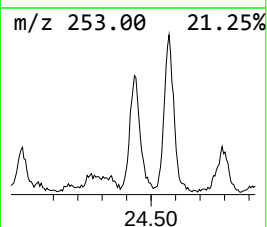
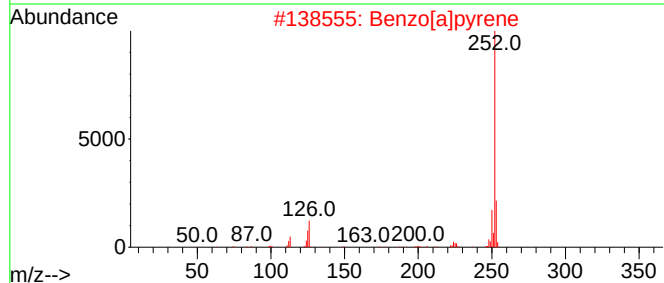
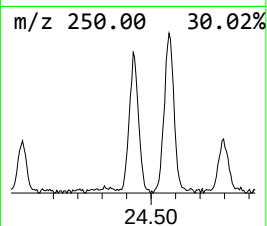
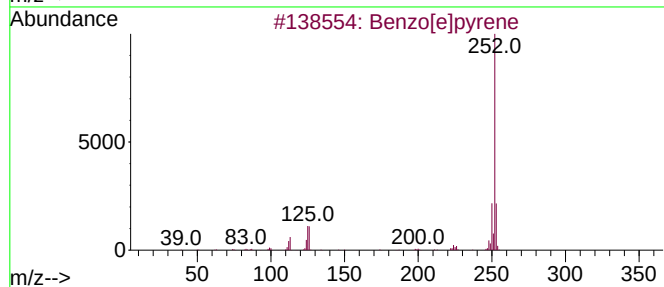
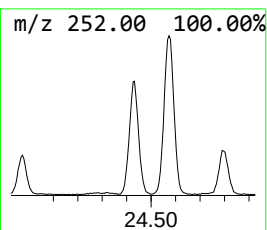
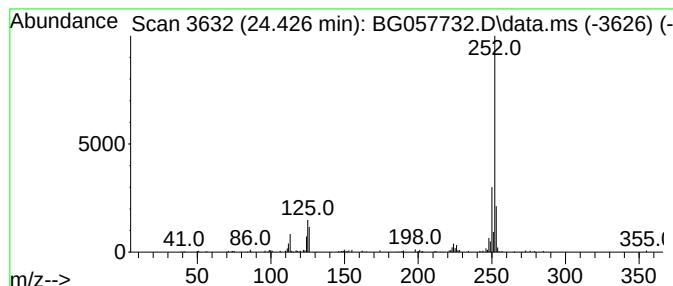
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.426	8.12 ng	261273	Perylene-d12	24.726

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[a]pyrene	252	C20H12	000050-32-8	95
3			Perylene	252	C20H12	000198-55-0	95
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061523\
Data File : BG057732.D
Acq On : 15 Jun 2023 20:16
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Sample : 03222-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

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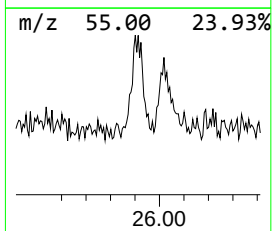
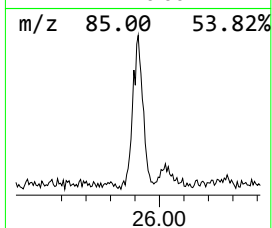
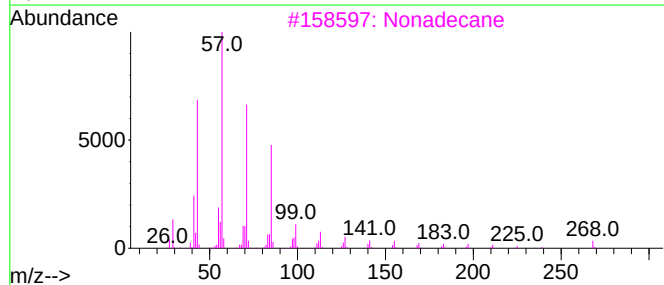
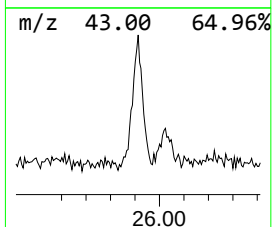
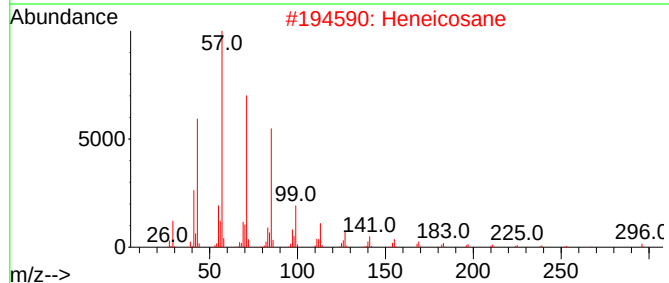
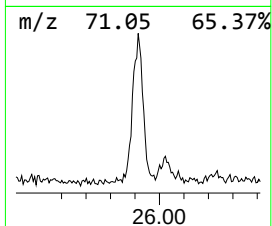
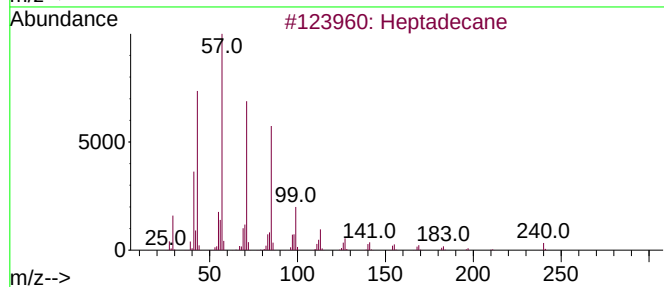
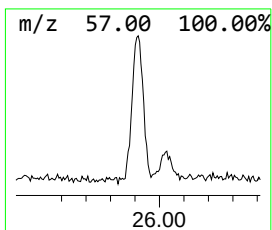
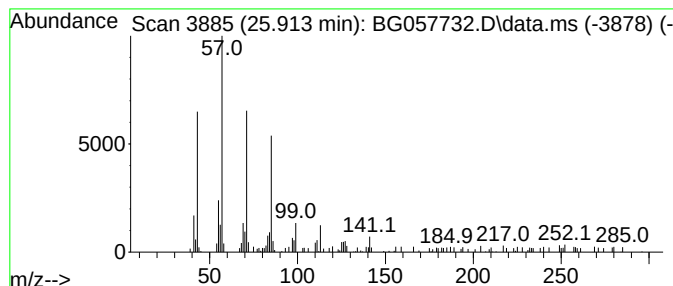
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.913	4.13 ng	132900	Perylene-d12	24.726

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	97
2		Heneicosane	296	C21H44	000629-94-7	93
3		Nonadecane	268	C19H40	000629-92-5	87
4		Octadecane	254	C18H38	000593-45-3	86
5		Hexadecane	226	C16H34	000544-76-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061523\
Data File : BG057732.D
Acq On : 15 Jun 2023 20:16
Operator : CG/JU
Sample : 03222-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-...	5.049	3.7	ng	48727	1	7.934	261006	20.0
Benzophenone	15.919	5.9	ng	134187	3	14.567	458231	20.0
Phenanthrene, 1...	18.233	2.3	ng	66954	4	17.311	571570	20.0
4H-Cyclopenta[d...	18.380	3.3	ng	94708	4	17.311	571570	20.0
unknown21.230	21.230	3.4	ng	172010	5	21.565	1014680	20.0
Supraene	23.245	3.6	ng	116327	6	24.726	643849	20.0
Triacontane	23.851	3.8	ng	123686	6	24.726	643849	20.0
Benzo[e]pyrene	24.426	8.1	ng	261273	6	24.726	643849	20.0
Heptadecane	25.913	4.1	ng	132900	6	24.726	643849	20.0