

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
 Data File : BG057773.D
 Acq On : 20 Jun 2023 12:47
 Operator : CG/JU
 Sample : 03262-07
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WS-SOIL3-0615

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-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057773.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.034	325	331	342	rVB	80249	121156	5.37%	0.779%
2	5.498	403	410	421	rBV	888012	1429785	63.36%	9.188%
3	7.090	671	681	688	rBV	871945	1506480	66.76%	9.681%
4	7.925	816	823	830	rBV	177990	298675	13.24%	1.919%
5	9.088	1012	1021	1029	rBV	516588	903135	40.02%	5.804%
6	10.727	1290	1300	1310	rVB	245824	429901	19.05%	2.763%
7	13.183	1711	1718	1726	rVB	1145382	1764493	78.20%	11.339%
8	14.558	1944	1952	1960	rVB	359170	562084	24.91%	3.612%
9	15.915	2177	2183	2188	rBV	53906	76322	3.38%	0.490%
10	16.045	2198	2205	2212	rBV	978756	1469696	65.13%	9.445%
11	17.302	2413	2419	2424	rBV	455092	679453	30.11%	4.366%
12	17.343	2424	2426	2432	rVB	58514	69691	3.09%	0.448%
13	18.189	2563	2570	2574	rBV2	145010	231105	10.24%	1.485%
14	18.224	2574	2576	2581	rVB	39717	46503	2.06%	0.299%
15	18.371	2596	2601	2605	rBV3	35319	63328	2.81%	0.407%
16	18.407	2605	2607	2613	rVB	21156	26000	1.15%	0.167%
17	18.677	2648	2653	2656	rBV	22440	31927	1.41%	0.205%
18	18.718	2656	2660	2668	rVB10	13008	23376	1.04%	0.150%
19	19.088	2719	2723	2728	rBV	26936	43419	1.92%	0.279%
20	19.229	2743	2747	2754	rBV2	19534	38050	1.69%	0.245%
21	19.352	2764	2768	2773	rVB	130971	179031	7.93%	1.151%
22	19.464	2782	2787	2796	rBV4	52053	73282	3.25%	0.471%
23	19.717	2821	2830	2839	rBV	211419	355903	15.77%	2.287%
24	19.787	2839	2842	2848	rVB7	13283	25015	1.11%	0.161%
25	19.916	2859	2864	2870	rBV	1660484	2256441	100.00%	14.501%
26	20.046	2880	2886	2890	rBV3	22828	50982	2.26%	0.328%
27	20.204	2904	2913	2920	rVB2	36826	105983	4.70%	0.681%
28	20.304	2928	2930	2936	rVB2	16155	24339	1.08%	0.156%
29	20.363	2936	2940	2944	rBV	39520	56707	2.51%	0.364%
30	20.504	2961	2964	2968	rBV	25941	29831	1.32%	0.192%
31	20.551	2968	2972	2976	rVB	35719	45130	2.00%	0.290%
32	20.721	2998	3001	3004	rVB	26007	27548	1.22%	0.177%
33	20.956	3038	3041	3049	rVB2	26868	52756	2.34%	0.339%
34	21.209	3077	3084	3092	rVV4	118448	211896	9.39%	1.362%
35	21.285	3093	3097	3105	rVB3	36329	61219	2.71%	0.393%
36	21.556	3134	3143	3147	rBV3	432275	850057	37.67%	5.463%

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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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.597	3147	3150	3158	rVB	86596	155608	6.90%	1.000%
38	21.756	3173	3177	3182	rVB4	30035	47497	2.10%	0.305%
39	22.349	3273	3278	3286	rVB5	31775	71826	3.18%	0.462%
40	23.700	3502	3508	3516	rBV4	35222	118570	5.25%	0.762%
41	24.411	3624	3629	3638	rVB2	28128	72776	3.23%	0.468%
42	24.546	3647	3652	3661	rVB	38827	93702	4.15%	0.602%
43	24.705	3669	3679	3697	rVB	271737	780351	34.58%	5.015%

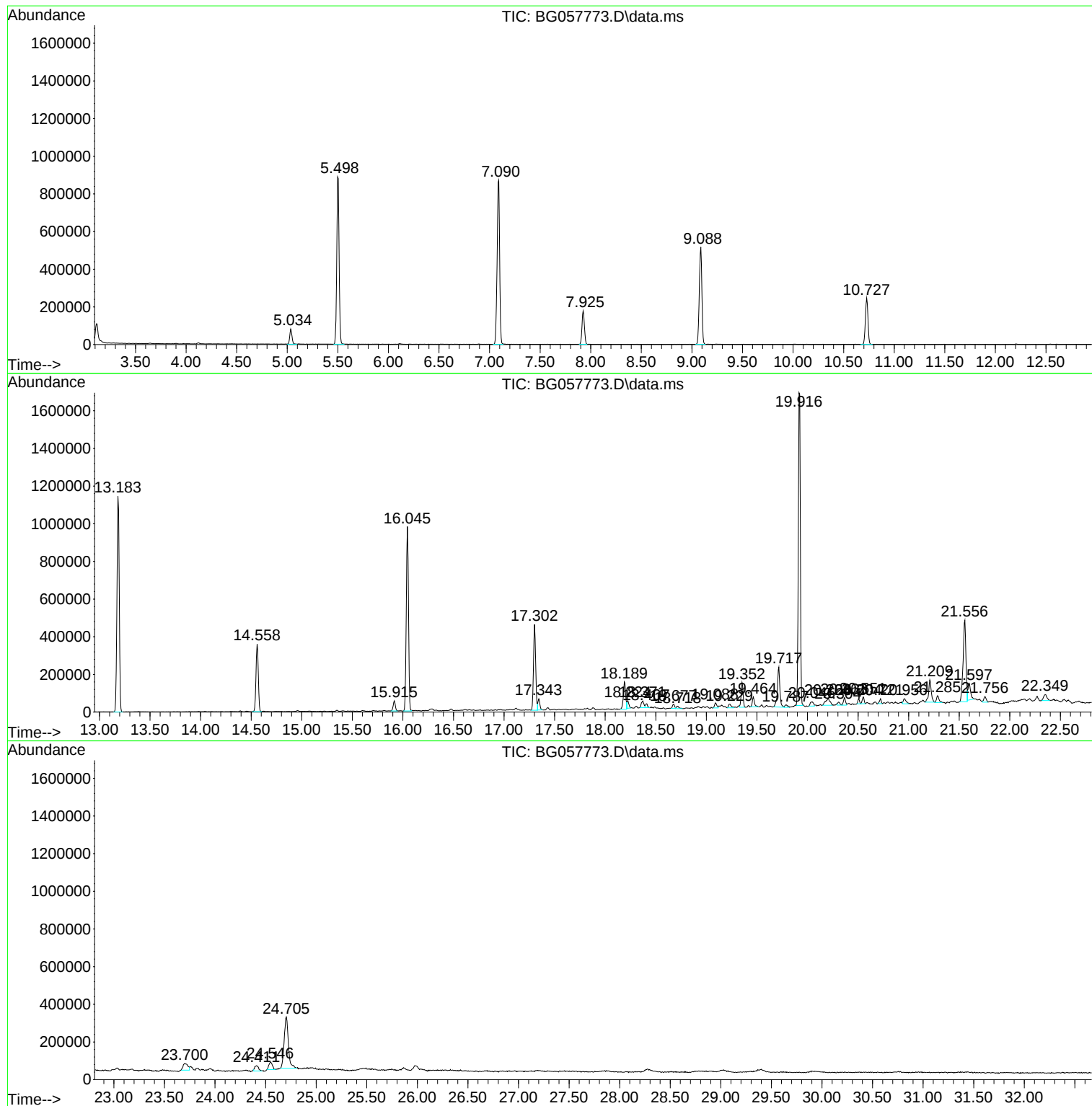
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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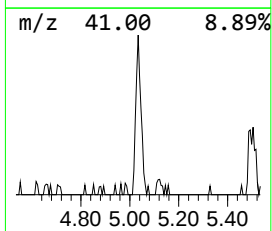
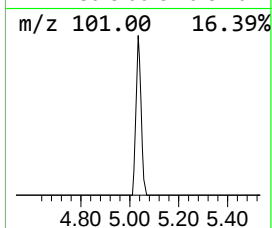
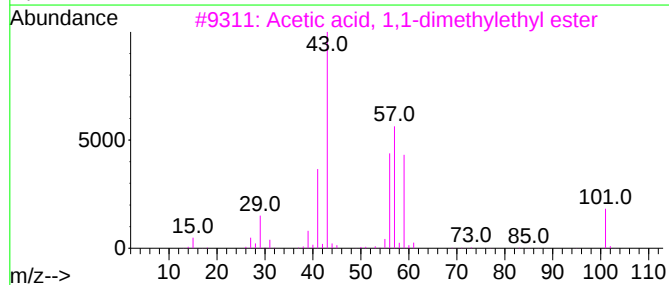
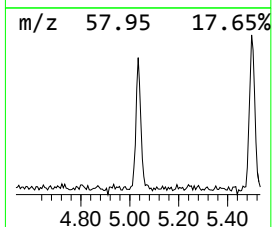
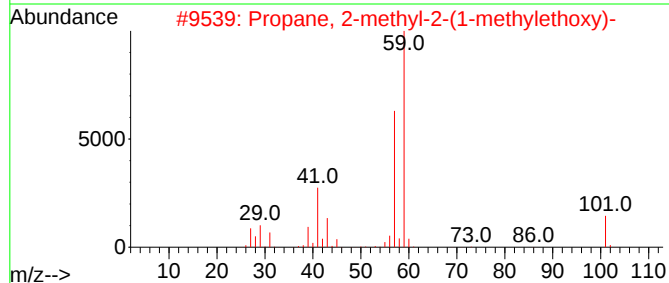
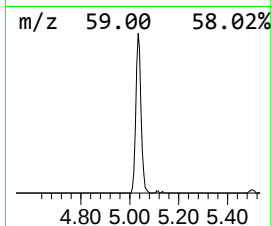
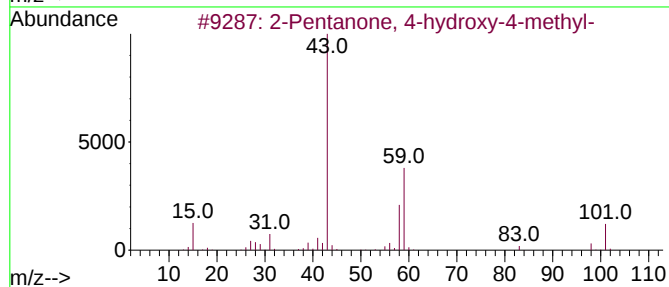
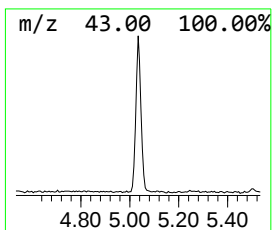
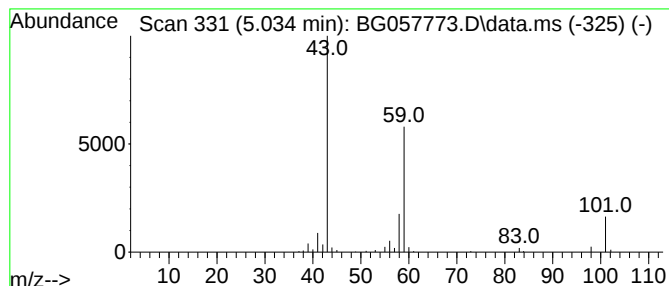
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	8.11 ng	121156	1,4-Dichlorobenzene-d4	7.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		



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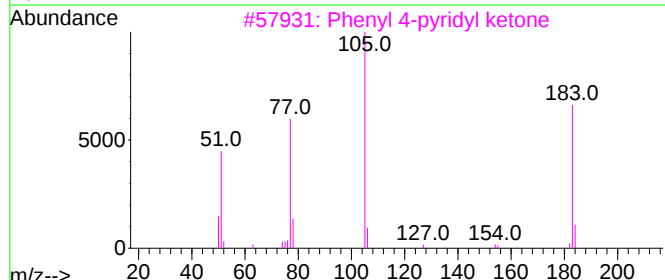
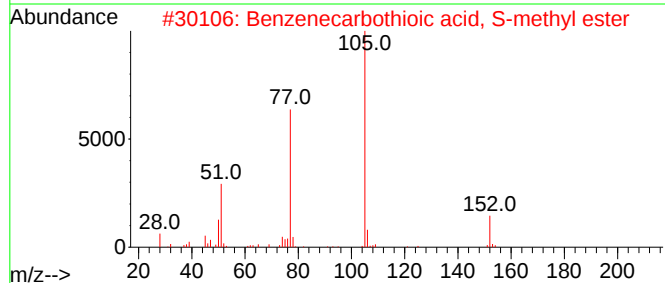
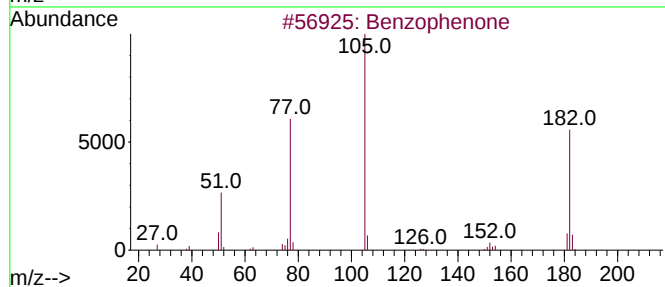
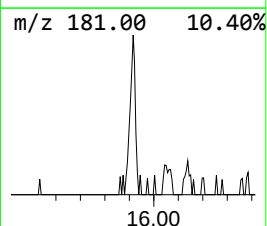
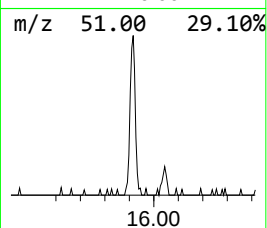
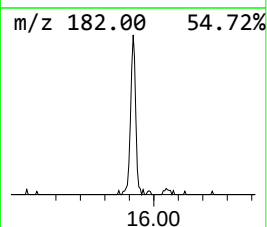
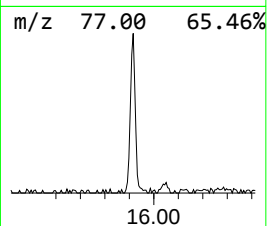
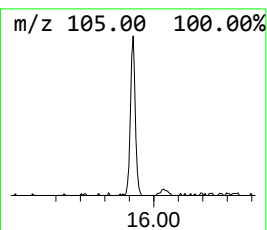
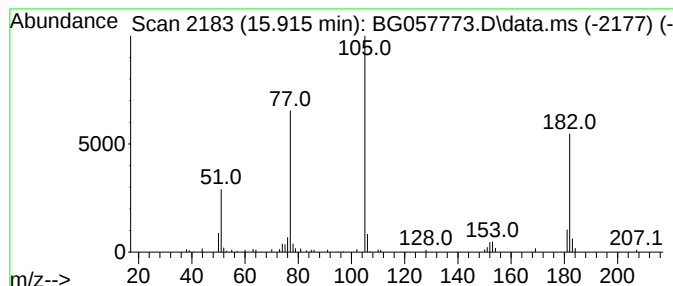
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.915	2.72 ng	76322	Acenaphthene-d10	14.558

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	47
4			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	46
5			Benzoylformic acid	150	C8H6O3	000611-73-4	46



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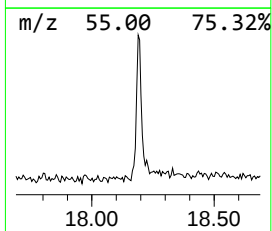
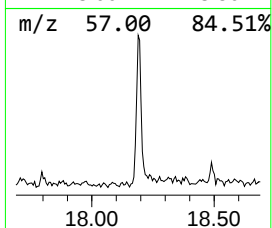
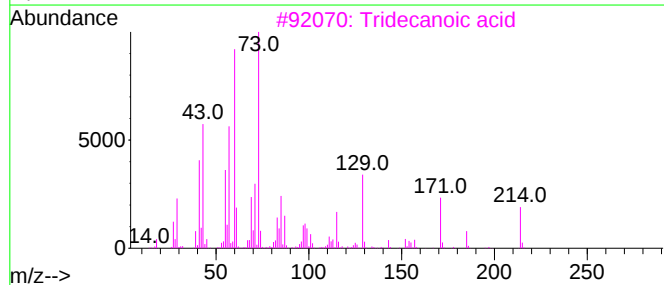
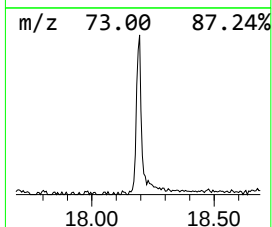
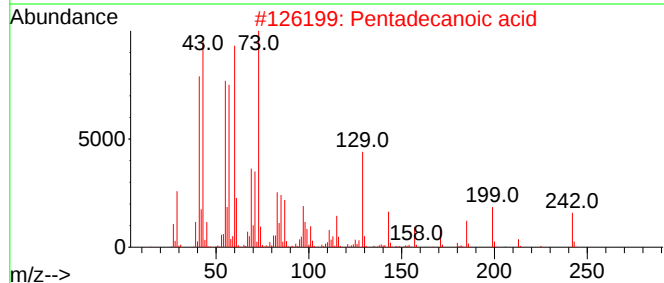
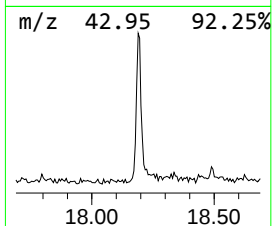
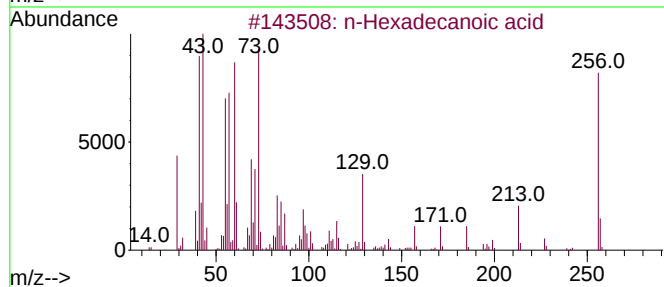
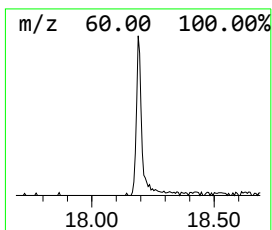
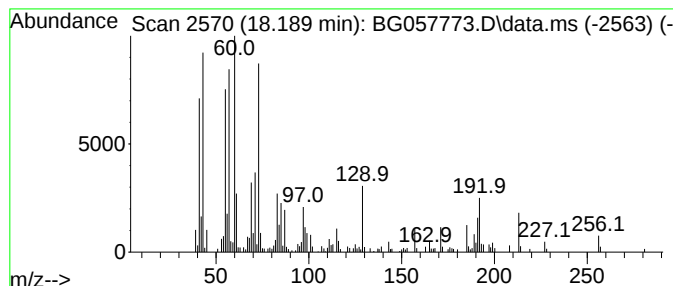
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.189	6.80 ng	231105	Phenanthrene-d10	17.302

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3			Tridecanoic acid	214	C13H26O2	000638-53-9	64
4			Undecanoic acid	186	C11H22O2	000112-37-8	59
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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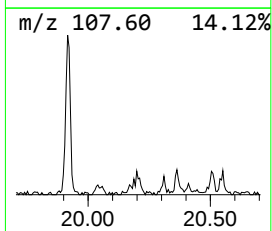
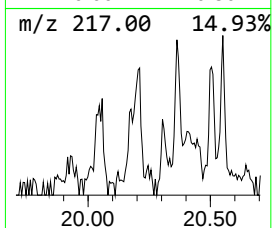
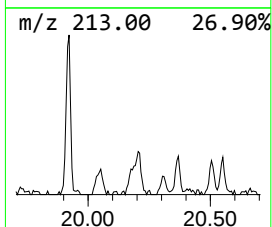
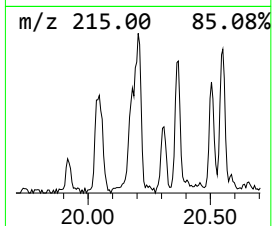
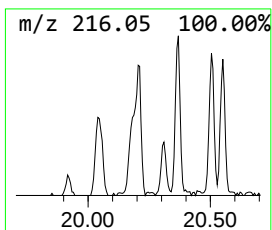
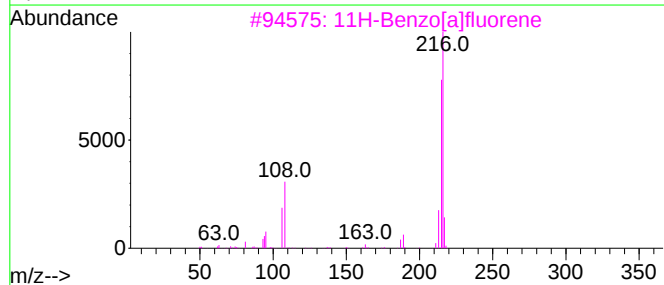
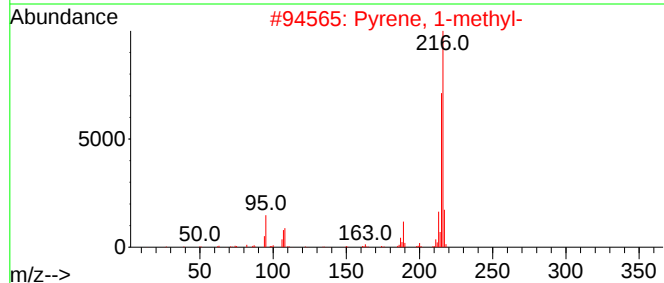
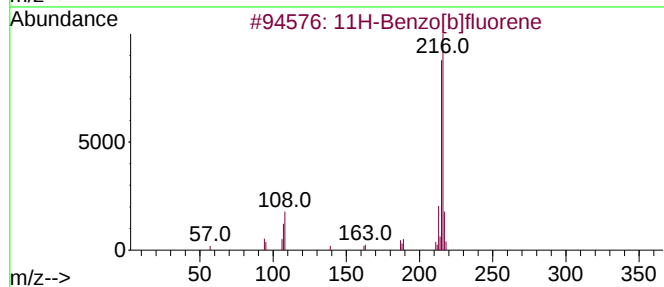
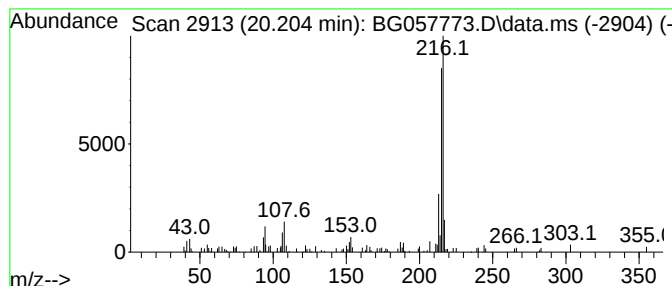
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Peak Number 4 11H-Benzo[b]fluorene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.204	2.49 ng	105983	Chrysene-d12	21.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
2		Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81
4		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81
5		Pyrene, 2-methyl-	216	C17H12	003442-78-2	76



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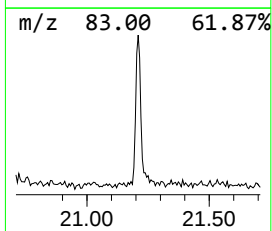
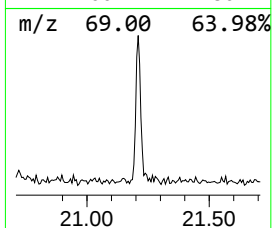
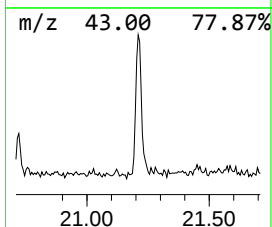
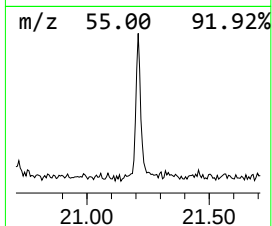
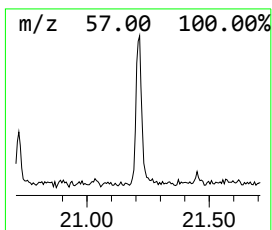
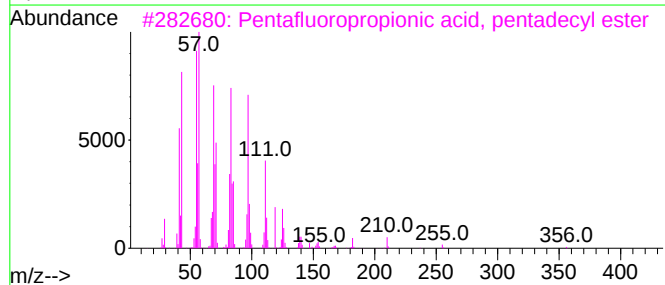
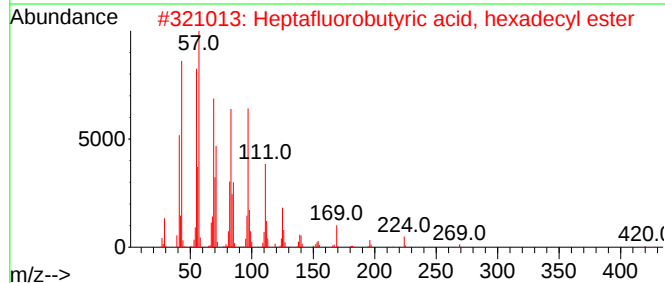
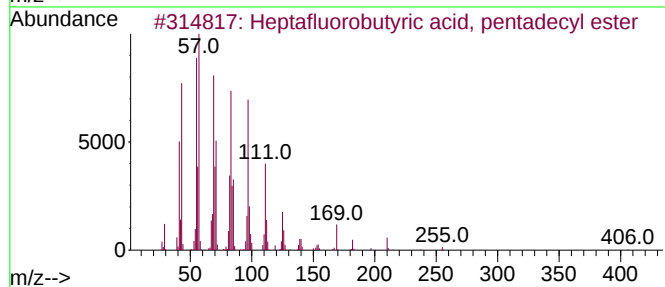
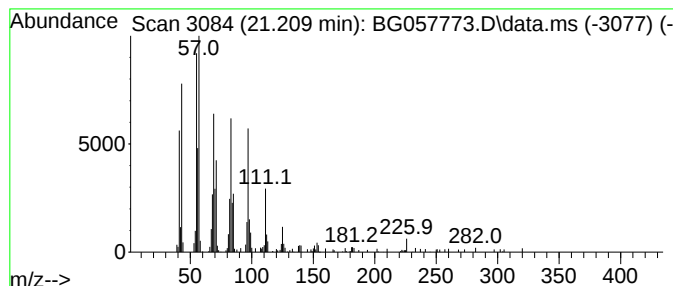
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptafluorobutyric acid, pe... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.209	4.99 ng	211896	Chrysene-d12	21.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
2			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
5			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
Data File : BG057773.D
Acq On : 20 Jun 2023 12:47
Operator : CG/JU
Sample : 03262-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WS-SOIL3-0615

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.034	8.1	ng	121156	1	7.925	298675	20.0
Benzophenone	15.915	2.7	ng	76322	3	14.558	562084	20.0
n-Hexadecanoic ...	18.189	6.8	ng	231105	4	17.302	679453	20.0
11H-Benzo[b]flu...	20.204	2.5	ng	105983	5	21.556	850057	20.0
Heptafluorobuty...	21.209	5.0	ng	211896	5	21.556	850057	20.0