

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112222\
 Data File : BG055748.D
 Acq On : 22 Nov 2022 20:40
 Operator : CG/JU
 Sample : N5718-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 VNJ-228

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-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055748.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.293	334	341	348	rBV	150002	230183	7.11%	1.134%
2	5.775	415	423	433	rBV	971262	1545114	47.70%	7.612%
3	7.391	690	698	709	rBV	954310	1661901	51.31%	8.188%
4	8.243	835	843	850	rBV	133991	225662	6.97%	1.112%
5	9.418	1034	1043	1054	rVB	552182	1013526	31.29%	4.993%
6	11.069	1315	1324	1333	rBV	197186	351862	10.86%	1.734%
7	13.489	1728	1736	1744	rBV	1486866	2370057	73.17%	11.677%
8	14.864	1962	1970	1976	rBV	332597	520013	16.05%	2.562%
9	14.929	1976	1981	1988	rVB	68726	107973	3.33%	0.532%
10	15.258	2028	2037	2044	rBV	38006	68911	2.13%	0.340%
11	15.904	2138	2147	2155	rBV2	71514	120133	3.71%	0.592%
12	16.210	2192	2199	2206	rVB2	100180	164368	5.07%	0.810%
13	16.351	2216	2223	2231	rBV	1330566	2096475	64.72%	10.329%
14	17.326	2385	2389	2393	rBV	29321	40639	1.25%	0.200%
15	17.426	2402	2406	2412	rVB2	26507	38482	1.19%	0.190%
16	17.608	2430	2437	2440	rBV	408876	633187	19.55%	3.120%
17	17.649	2440	2444	2450	rVB	380966	556414	17.18%	2.741%
18	17.737	2451	2459	2463	rBV	97465	164587	5.08%	0.811%
19	18.002	2501	2504	2512	rVB	25117	37032	1.14%	0.182%
20	18.466	2578	2583	2589	rBV2	296686	447839	13.83%	2.206%
21	18.525	2589	2593	2598	rVB	60557	102331	3.16%	0.504%
22	18.678	2613	2619	2623	rBV3	97093	178271	5.50%	0.878%
23	18.754	2629	2632	2640	rBV3	21225	40848	1.26%	0.201%
24	18.965	2664	2668	2672	rBV	37283	51656	1.59%	0.254%
25	19.007	2672	2675	2684	rVB2	29450	48134	1.49%	0.237%
26	19.377	2734	2738	2743	rBV3	53059	89644	2.77%	0.442%
27	19.524	2759	2763	2770	rBV2	31226	65190	2.01%	0.321%
28	19.647	2779	2784	2790	rVB	702534	986770	30.46%	4.862%
29	19.723	2793	2797	2803	rBV2	94061	160140	4.94%	0.789%
30	19.976	2836	2840	2841	rBV2	87173	112494	3.47%	0.554%
31	20.005	2841	2845	2853	rVB	531637	797624	24.62%	3.930%
32	20.193	2872	2877	2883	rVB	2495635	3239130	100.00%	15.958%
33	21.504	3097	3100	3105	rBV2	111376	169576	5.24%	0.835%
34	21.903	3161	3168	3173	rBV2	423930	971451	29.99%	4.786%
35	21.950	3174	3176	3183	rVB	196820	279301	8.62%	1.376%
36	25.311	3741	3748	3758	rVB2	219967	610328	18.84%	3.007%

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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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

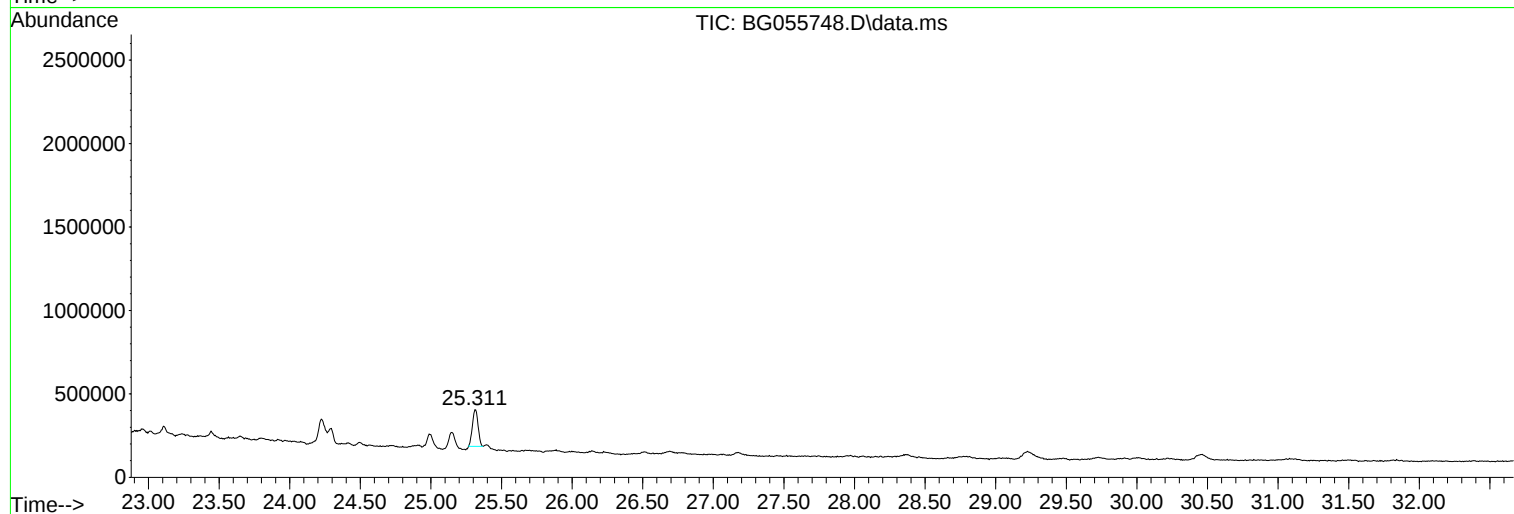
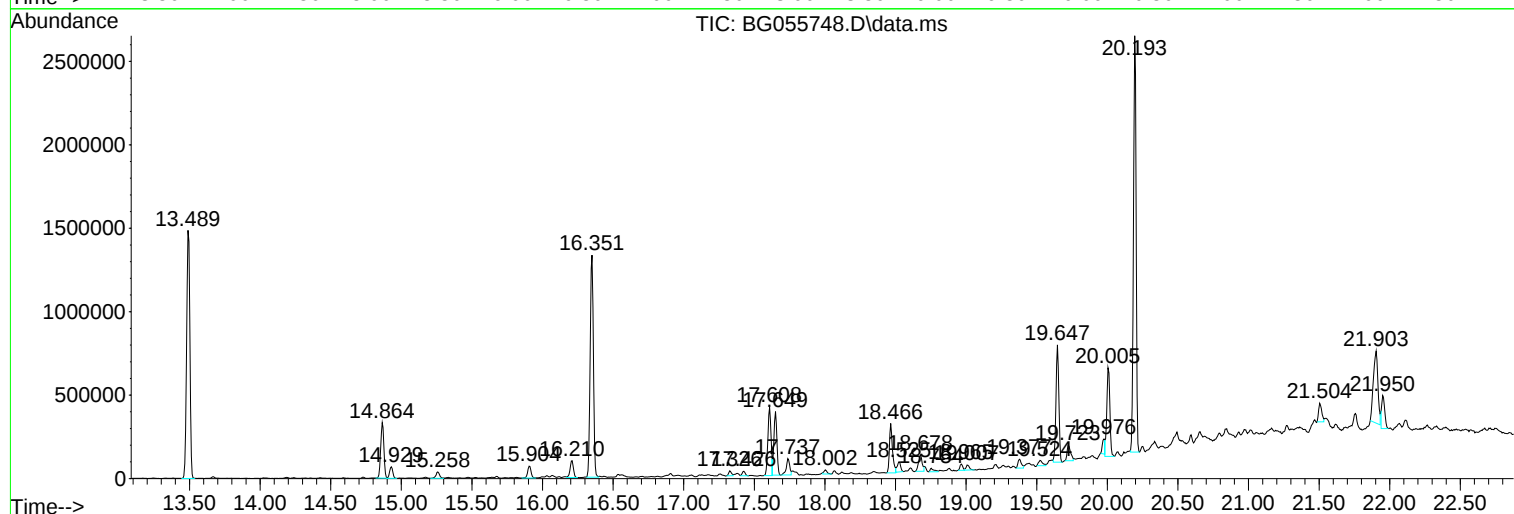
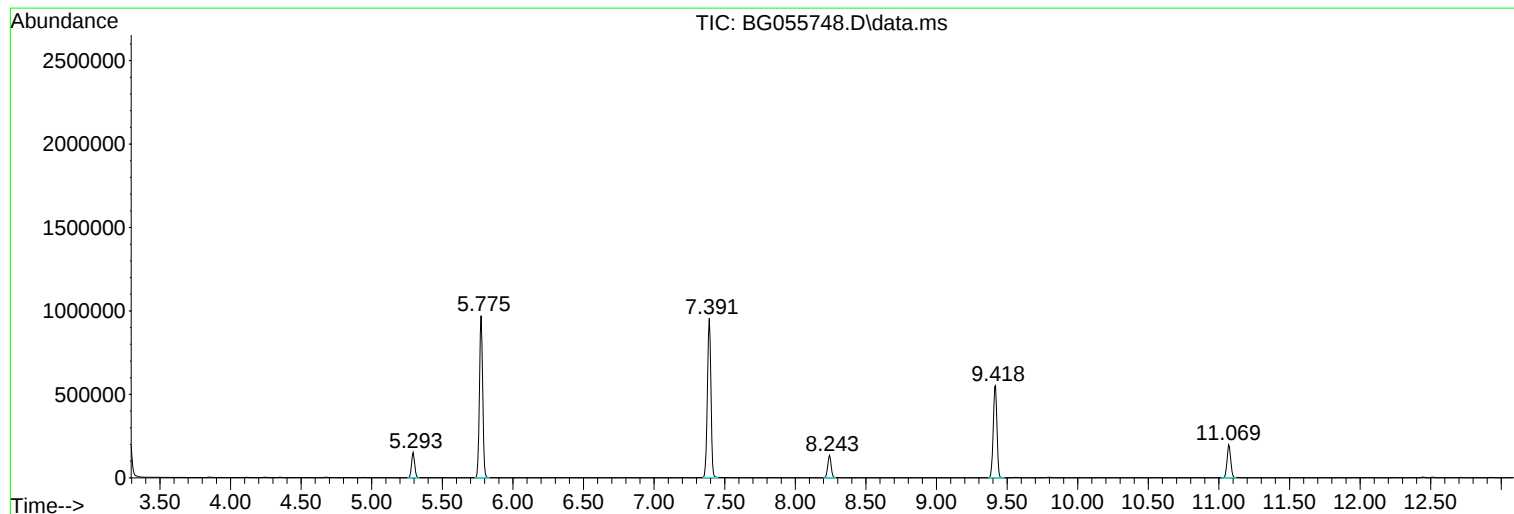
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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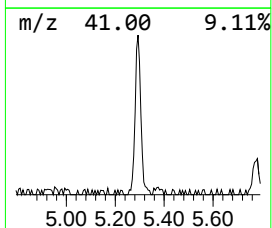
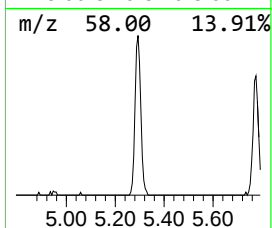
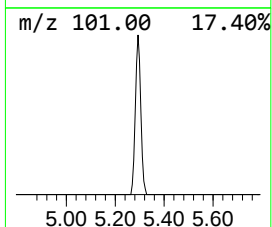
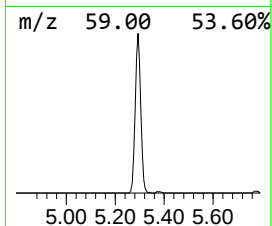
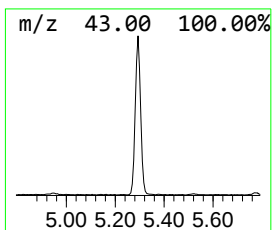
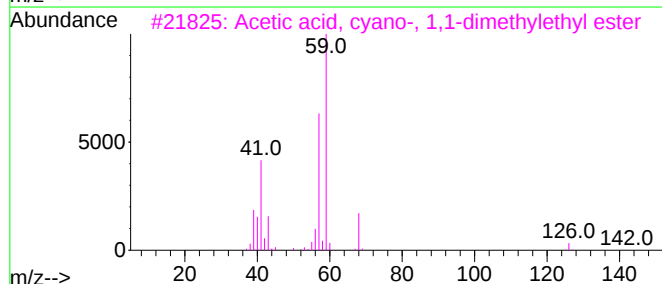
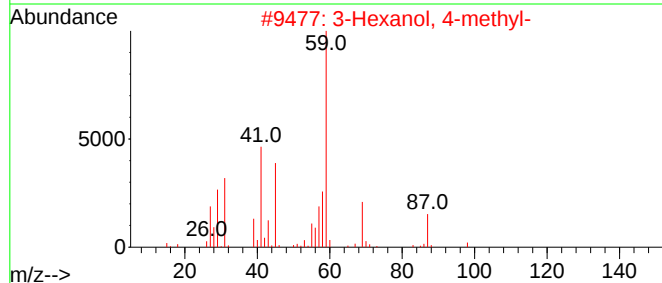
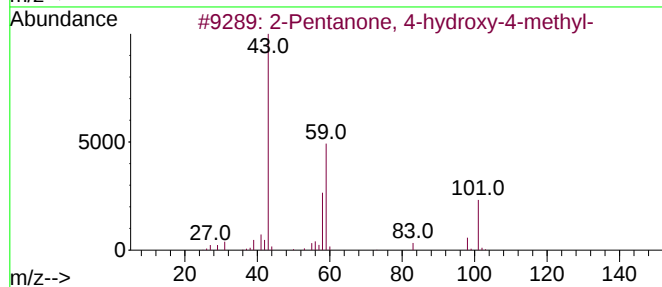
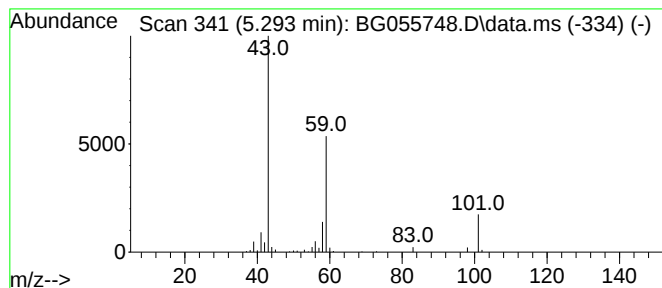
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.293	20.40 ng	230183	1,4-Dichlorobenzene-d4	8.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		



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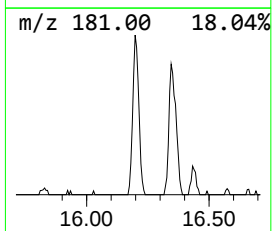
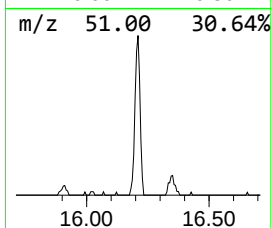
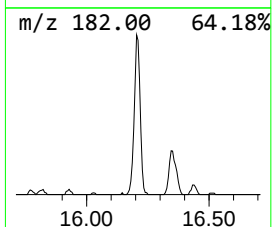
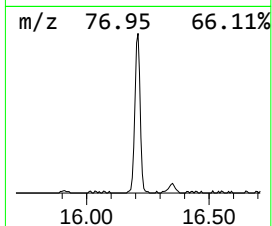
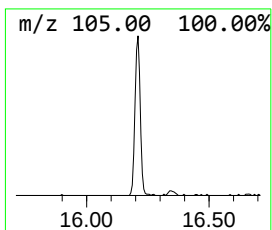
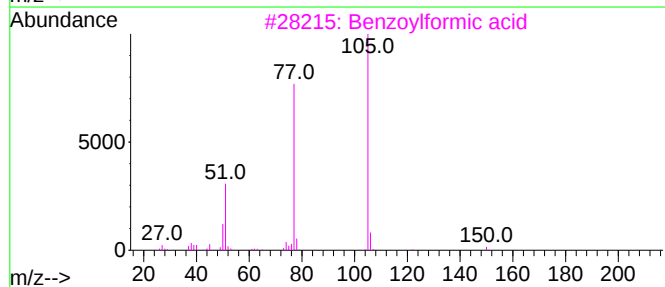
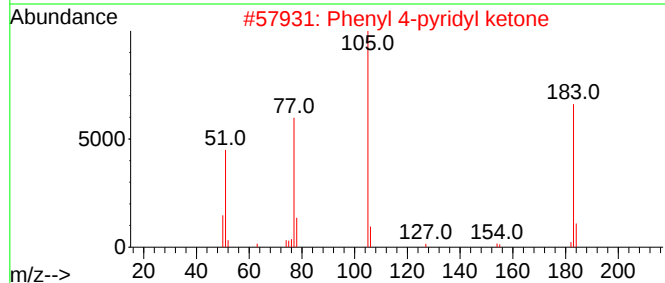
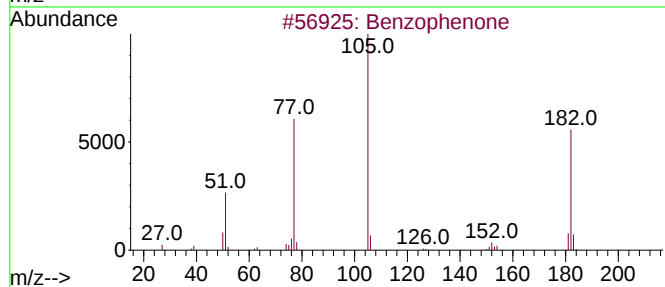
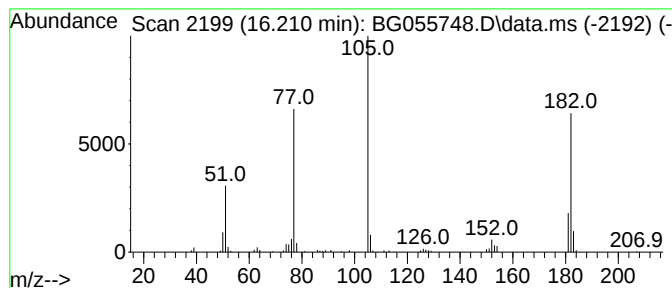
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.210	6.32 ng	164368	Acenaphthene-d10	14.864

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3			Benzoylformic acid	150	C8H6O3	000611-73-4	49
4			Vinyl benzoate	148	C9H8O2	000769-78-8	47
5			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47



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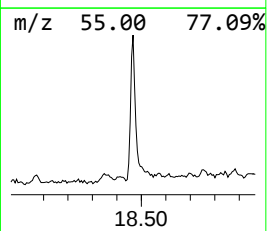
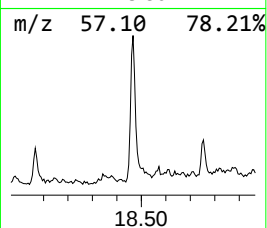
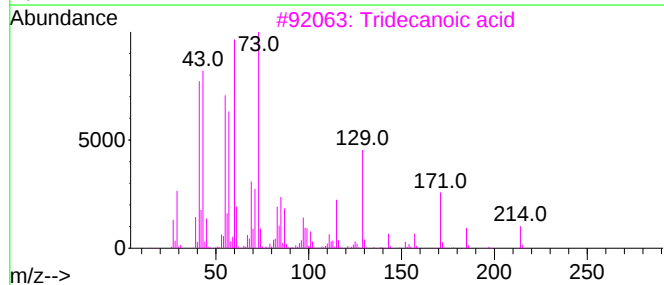
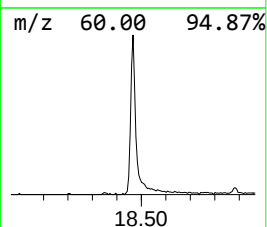
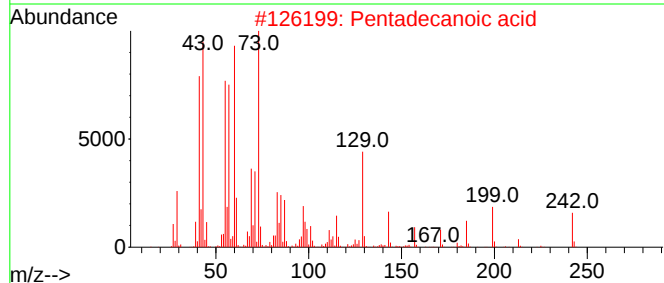
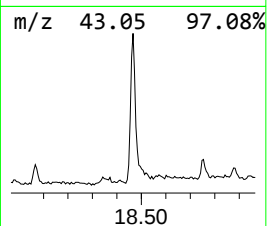
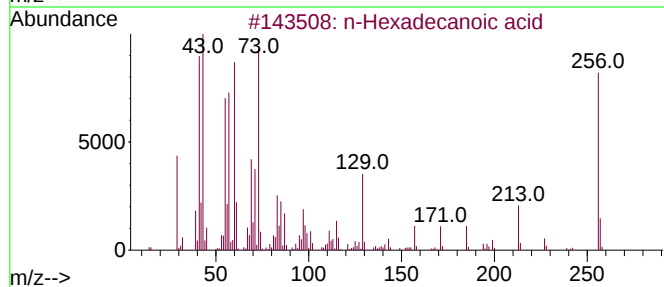
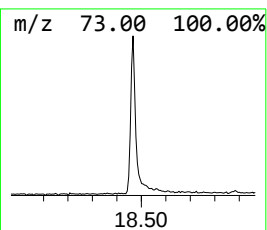
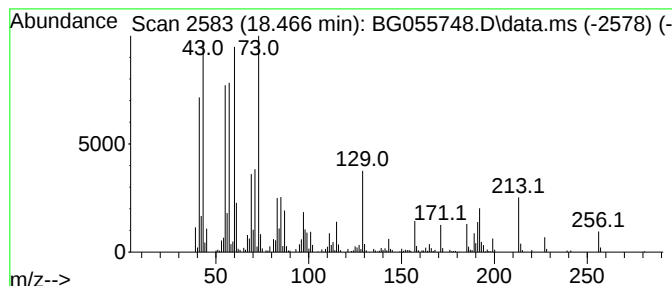
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.466	14.15 ng	447839	Phenanthrene-d10	17.608

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	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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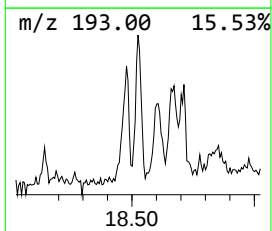
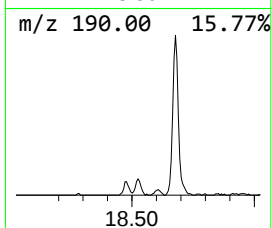
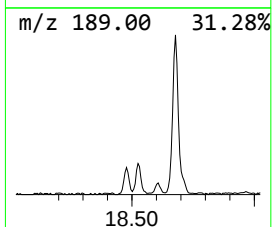
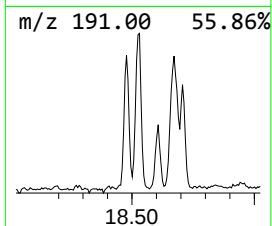
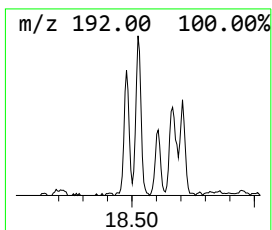
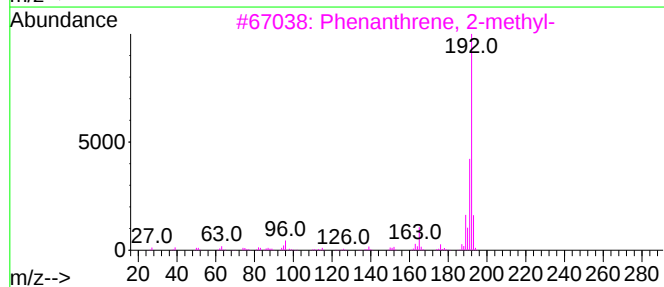
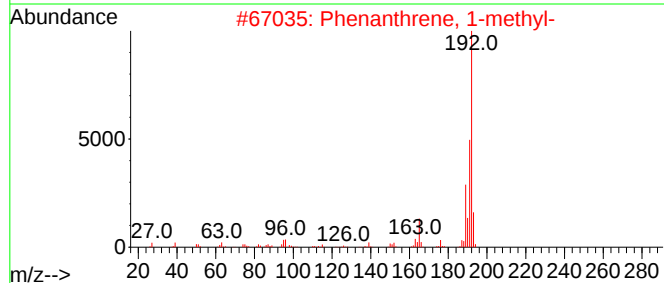
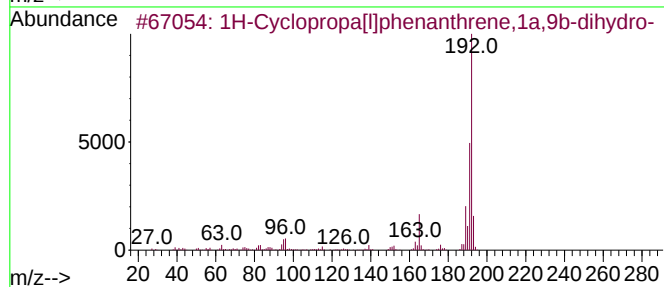
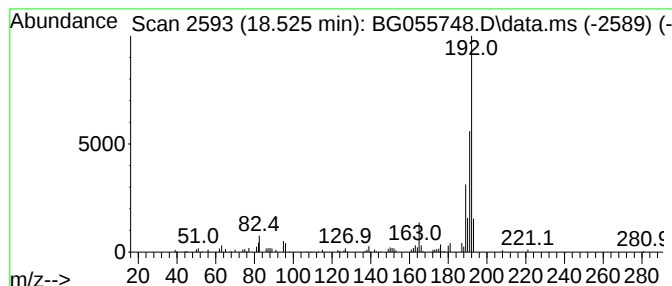
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1H-Cyclopropa[l]phenanthren... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.525	3.23 ng	102331	Phenanthrene-d10		17.608	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1H-Cyclopropa[1]phenanthrene,1a,...		192	C15H12	000949-41-7	96
2	Phenanthrene, 1-methyl-		192	C15H12	000832-69-9	96
3	Phenanthrene, 2-methyl-		192	C15H12	002531-84-2	95
4	1H-Indene, 2-phenyl-		192	C15H12	004505-48-0	94
5	Anthracene, 1-methyl-		192	C15H12	000610-48-0	93



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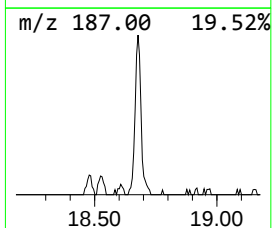
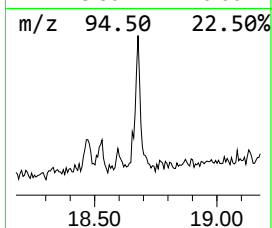
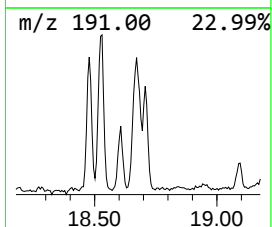
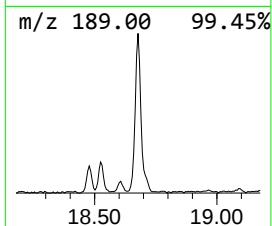
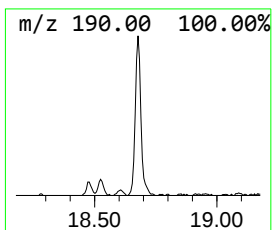
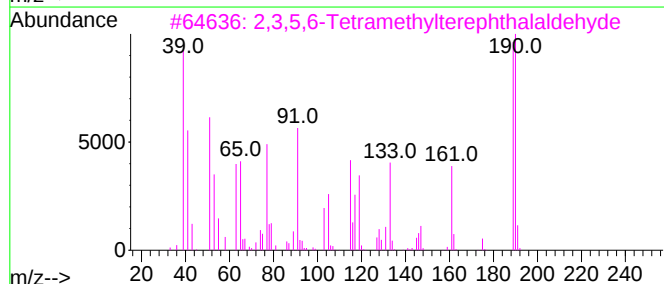
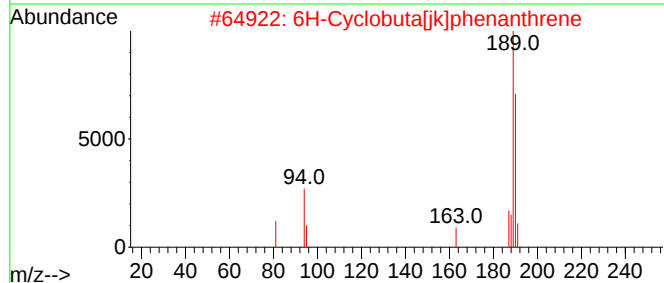
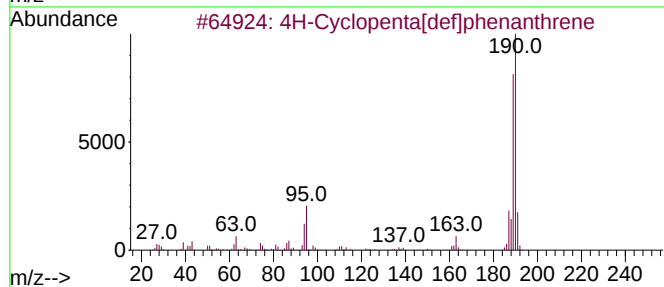
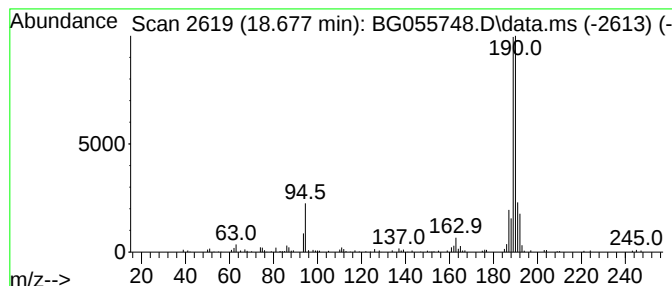
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.677	5.63 ng	178271	Phenanthrene-d10	17.608	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	91
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112222\
Data File : BG055748.D
Acq On : 22 Nov 2022 20:40
Operator : CG/JU
Sample : N5718-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-228

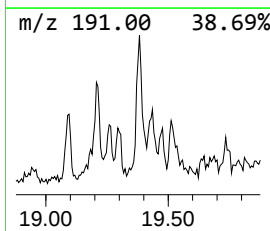
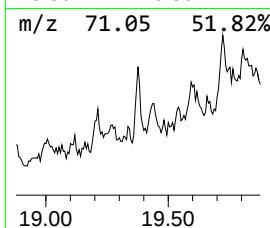
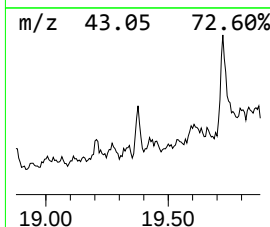
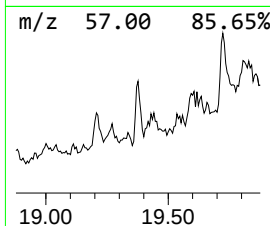
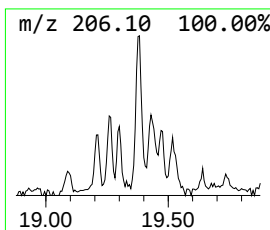
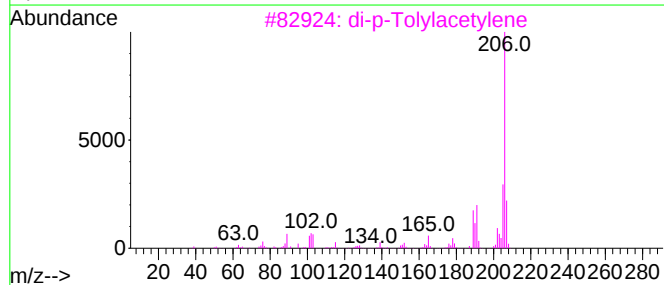
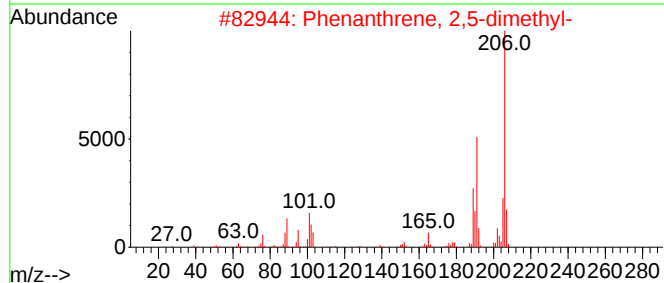
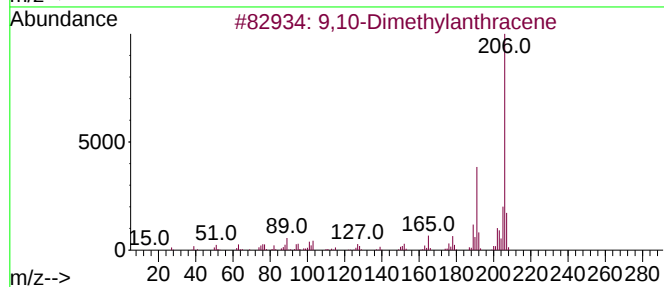
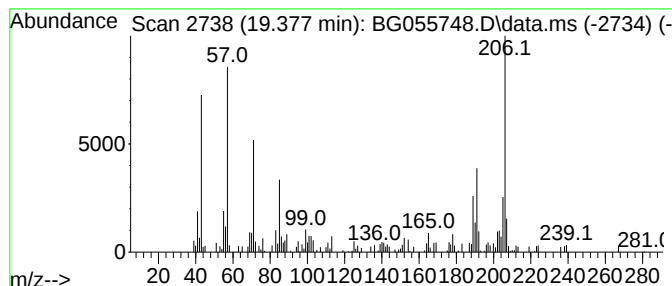
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9,10-Dimethylantracene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.377	2.83 ng	89644	Phenanthrene-d10	17.608

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,10-Dimethylantracene	206	C16H14	000781-43-1	95
2			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
3			di-p-Tolylacetylene	206	C16H14	002789-88-0	90
4			Naphthalene, 1,2-dihydro-1-phenyl-	206	C16H14	016606-46-5	89
5			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112222\
Data File : BG055748.D
Acq On : 22 Nov 2022 20:40
Operator : CG/JU
Sample : N5718-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

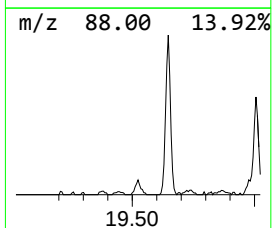
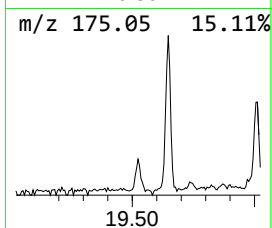
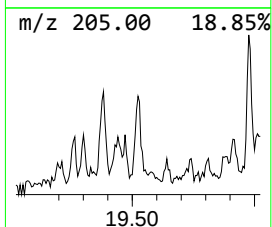
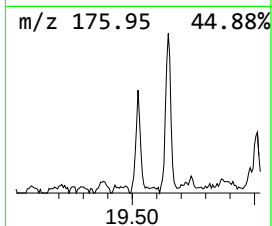
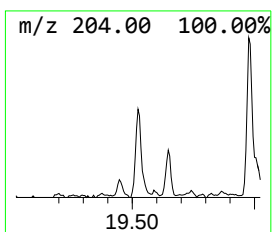
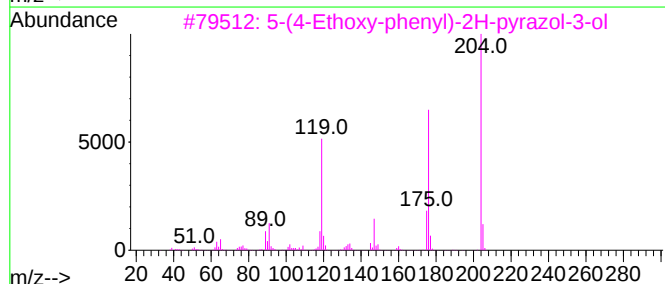
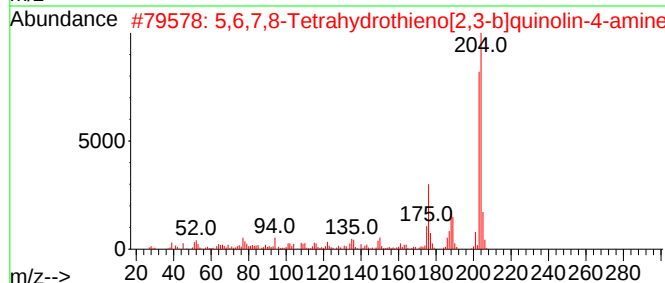
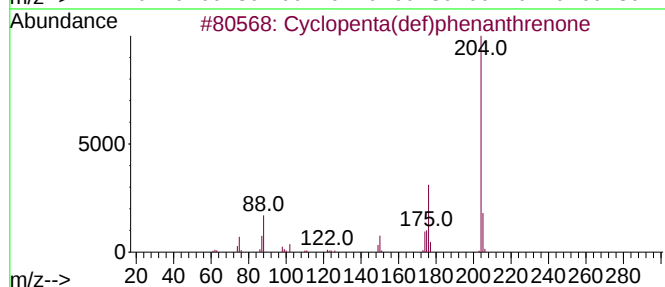
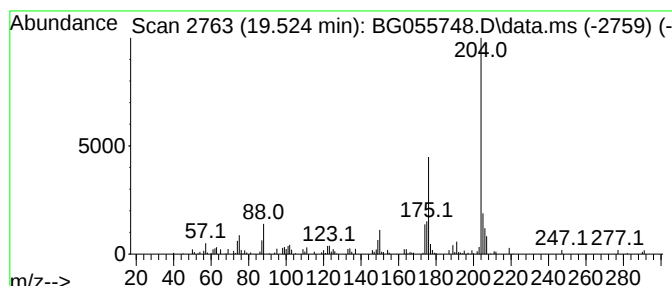
Instrument :
BNA_G
ClientSampleId :
VNJ-228

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclopenta(def)phenanthrenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.524	2.06 ng	65190	Phenanthrene-d10	17.608	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	93
2	5,6,7,8-Tetrahydrothieno[2,3-b]q...	204	C11H12N2S	122914-50-5	64
3	5-(4-Ethoxy-phenyl)-2H-pyrazol-3-ol	204	C11H12N2O2	1000278-26-8	53
4	Tetracyano-p-quinodimethane	204	C12H4N4	001518-16-7	43
5	4-Methyl-6,7-methylenedioxycoumarin	204	C11H8O4	015071-04-2	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112222\
Data File : BG055748.D
Acq On : 22 Nov 2022 20:40
Operator : CG/JU
Sample : N5718-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

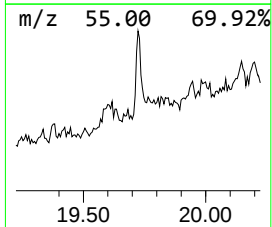
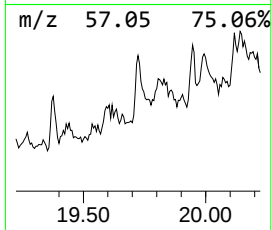
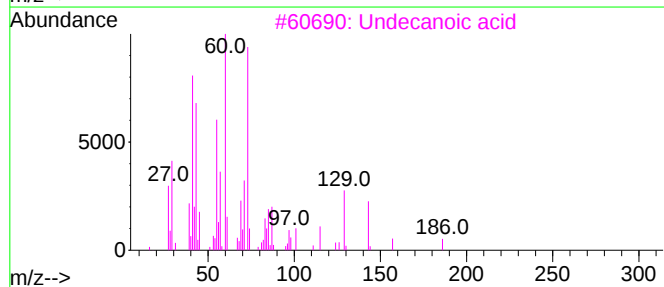
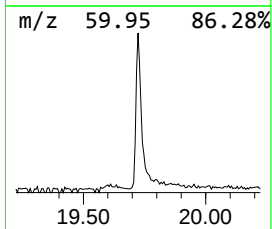
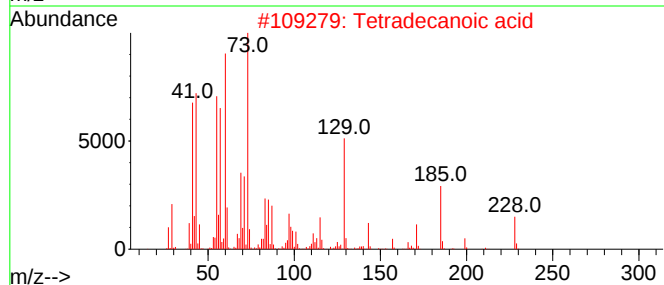
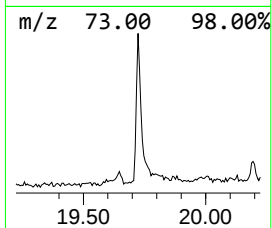
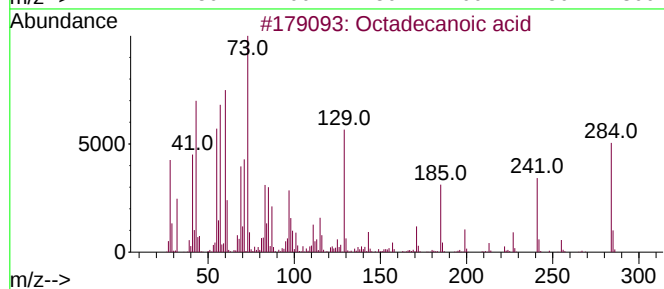
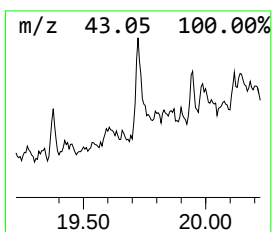
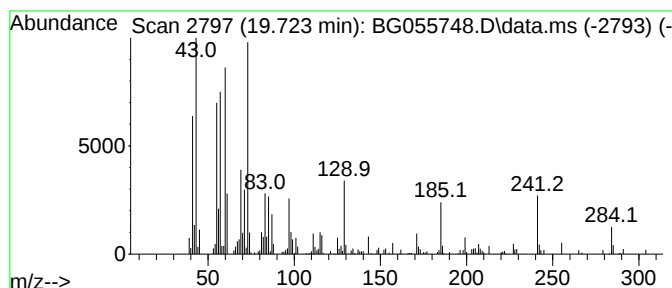
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.723	5.06 ng	160140	Phenanthrene-d10		17.608	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	97
2	Tetradecanoic acid		228	C14H28O2	000544-63-8	68
3	Undecanoic acid		186	C11H22O2	000112-37-8	55
4	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	53
5	Tridecanoic acid		214	C13H26O2	000638-53-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112222\
Data File : BG055748.D
Acq On : 22 Nov 2022 20:40
Operator : CG/JU
Sample : N5718-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-228

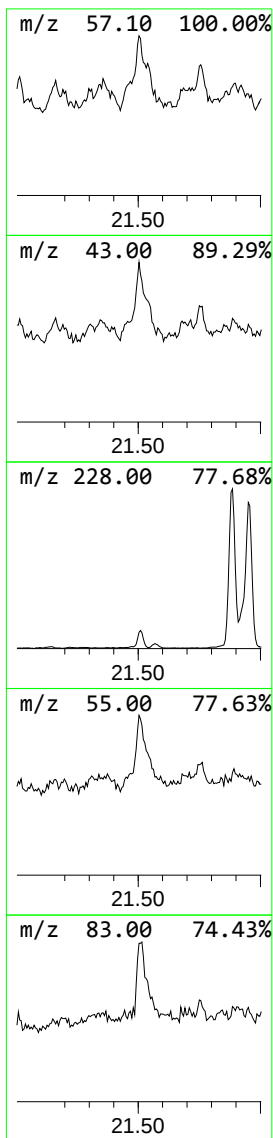
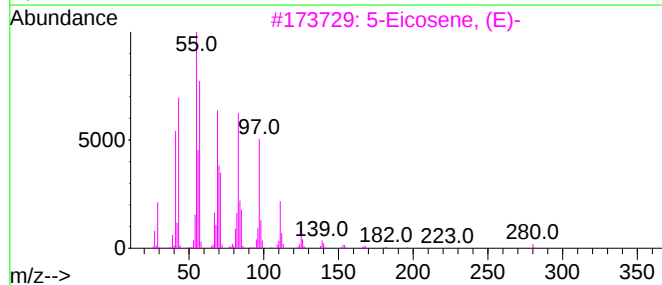
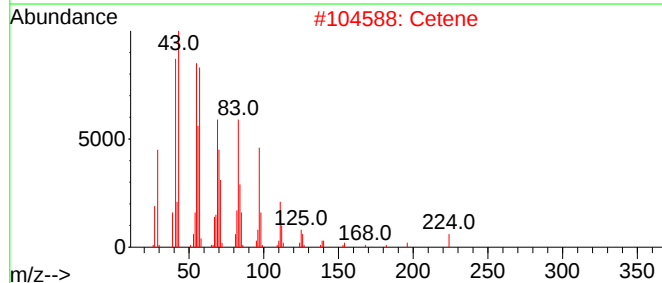
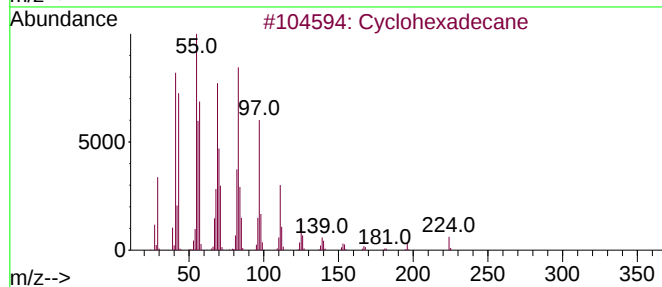
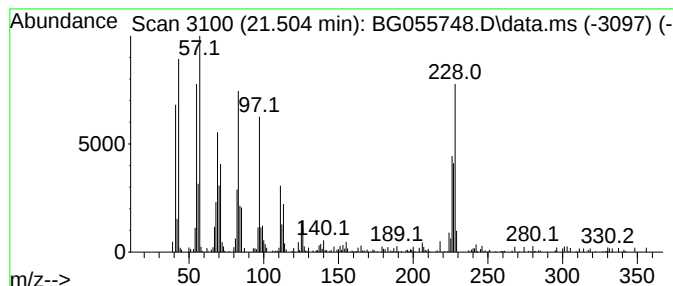
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.504	3.49 ng	169576	Chrysene-d12	21.903

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexadecane	224	C16H32	000295-65-8	84
2		Cetene	224	C16H32	000629-73-2	62
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	60
4		1-Heneicosanol	312	C21H44O	015594-90-8	59
5		1-Hexacosene	364	C26H52	018835-33-1	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112222\
Data File : BG055748.D
Acq On : 22 Nov 2022 20:40
Operator : CG/JU
Sample : N5718-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
VNJ-228

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
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
2-Pentanone, 4-...	5.293	20.4	ng	230183	1	8.243	225662	20.0
Benzophenone	16.210	6.3	ng	164368	3	14.864	520013	20.0
n-Hexadecanoic ...	18.466	14.2	ng	447839	4	17.608	633187	20.0
1H-Cyclopropa[l...	18.525	3.2	ng	102331	4	17.608	633187	20.0
4H-Cyclopenta[d...	18.677	5.6	ng	178271	4	17.608	633187	20.0
9,10-Dimethylan...	19.377	2.8	ng	89644	4	17.608	633187	20.0
Cyclopenta(def)...	19.524	2.1	ng	65190	4	17.608	633187	20.0
Octadecanoic acid	19.723	5.1	ng	160140	4	17.608	633187	20.0
Cyclohexadecane	21.504	3.5	ng	169576	5	21.903	971451	20.0