

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100722\
 Data File : BG055102.D
 Acq On : 7 Oct 2022 16:53
 Operator : CG/JU
 Sample : N5022-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DSN003

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-BG100322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055102.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.376	9	15	43	rVB	557489	1000562	47.71%	10.438%
2	5.385	349	357	368	rBV	48217	79966	3.81%	0.834%
3	5.855	430	437	452	rVB	196506	337817	16.11%	3.524%
4	7.459	703	710	722	rBV	131849	229386	10.94%	2.393%
5	8.334	853	859	872	rVB	81765	144904	6.91%	1.512%
6	9.504	1050	1058	1067	rBV	280235	496568	23.68%	5.180%
7	11.166	1331	1341	1347	rBV	121443	206666	9.85%	2.156%
8	13.570	1744	1750	1758	rBV	766969	1163497	55.48%	12.138%
9	14.939	1973	1983	1992	rVB	204488	308957	14.73%	3.223%
10	16.413	2227	2234	2241	rBV	788283	1197111	57.08%	12.488%
11	17.236	2369	2374	2382	rVB	21997	30431	1.45%	0.317%
12	17.671	2442	2448	2456	rBV	303887	455633	21.73%	4.753%
13	17.964	2495	2498	2505	rVB2	16173	24460	1.17%	0.255%
14	18.523	2585	2593	2601	rBV	74335	115155	5.49%	1.201%
15	18.593	2601	2605	2611	rVB2	20122	31138	1.48%	0.325%
16	19.780	2802	2807	2813	rBV2	48977	68360	3.26%	0.713%
17	20.138	2863	2868	2873	rVB	16253	21414	1.02%	0.223%
18	20.250	2881	2887	2893	rBV	1601711	2097177	100.00%	21.878%
19	21.037	3016	3021	3027	rBV5	13119	21231	1.01%	0.221%
20	21.572	3106	3112	3117	rBV3	41522	69694	3.32%	0.727%
21	21.966	3172	3179	3188	rVB	319244	533496	25.44%	5.565%
22	22.154	3206	3211	3218	rVB2	23434	36200	1.73%	0.378%
23	22.806	3316	3322	3328	rBV2	26558	50706	2.42%	0.529%
24	23.552	3444	3449	3455	rVB3	26204	48219	2.30%	0.503%
25	24.422	3591	3597	3605	rBV2	23218	50926	2.43%	0.531%
26	25.409	3754	3765	3782	rBV2	180246	600222	28.62%	6.261%
27	26.695	3977	3984	3993	rVB4	18339	51918	2.48%	0.542%
28	28.182	4230	4237	4248	rVB4	15136	54268	2.59%	0.566%
29	29.986	4533	4544	4560	rVB5	12915	59885	2.86%	0.625%

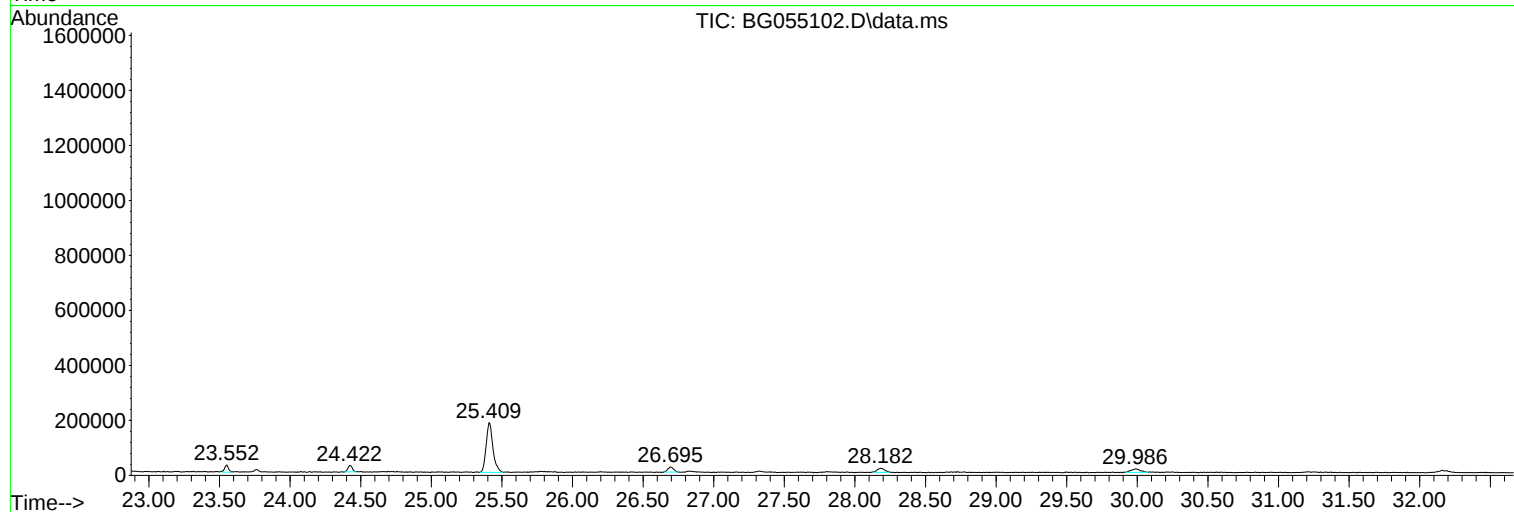
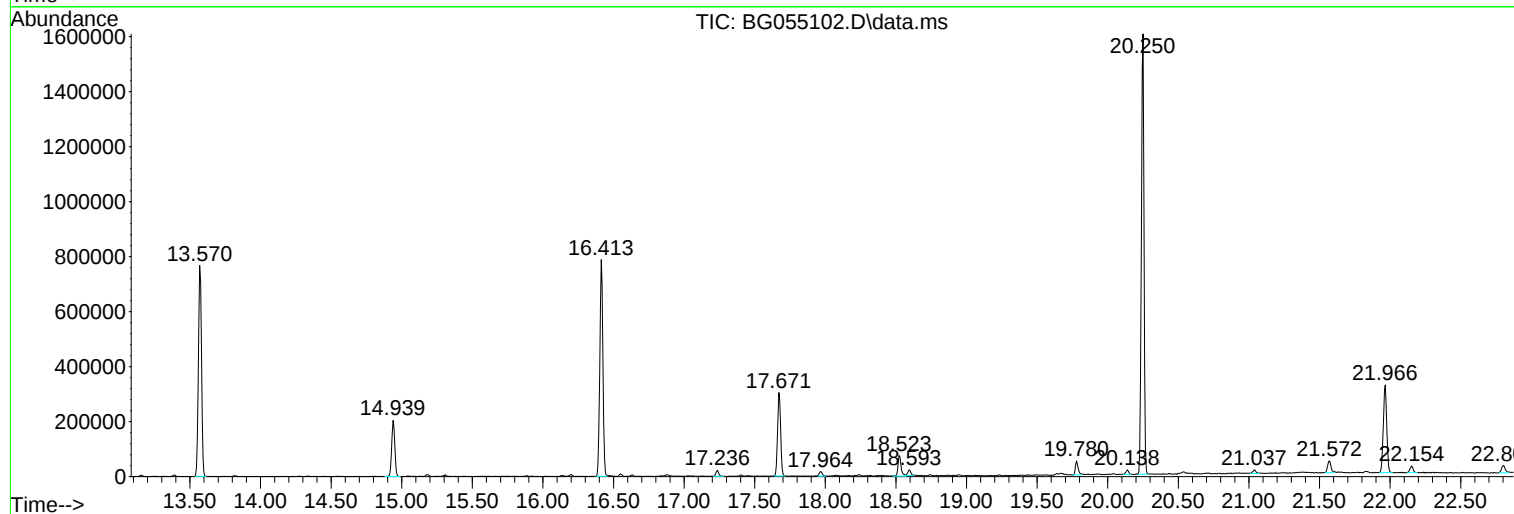
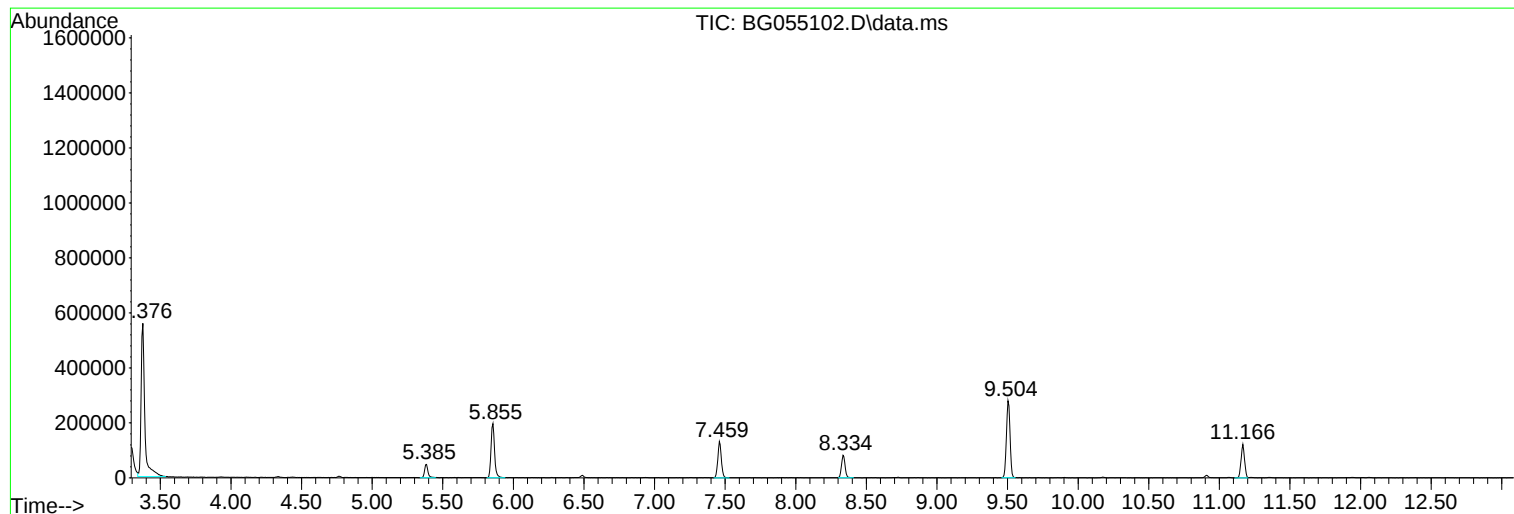
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DSN003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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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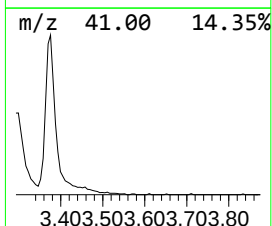
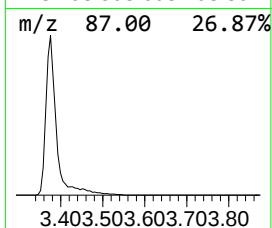
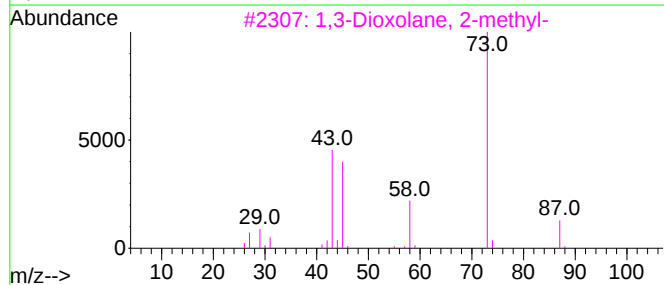
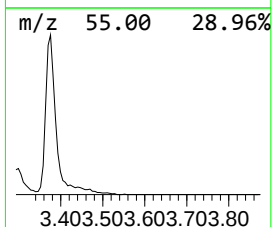
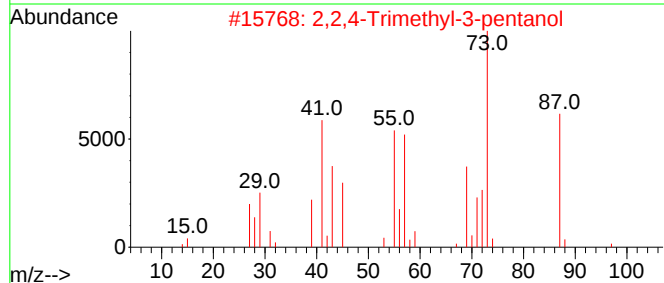
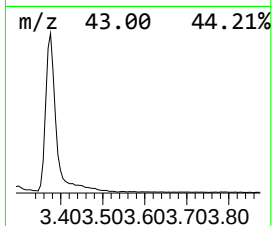
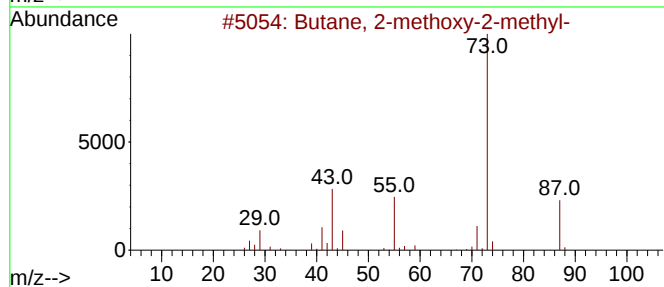
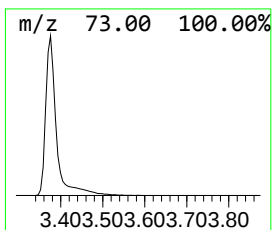
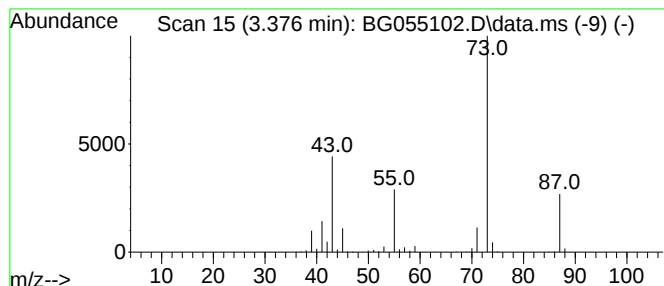
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.376	138.10 ng	1000560	1,4-Dichlorobenzene-d4	8.334

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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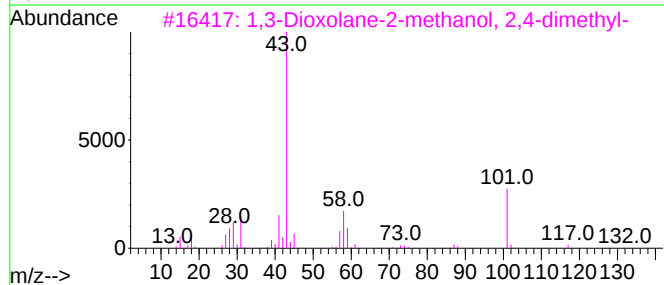
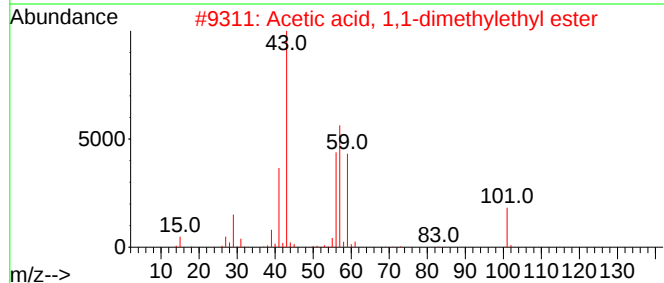
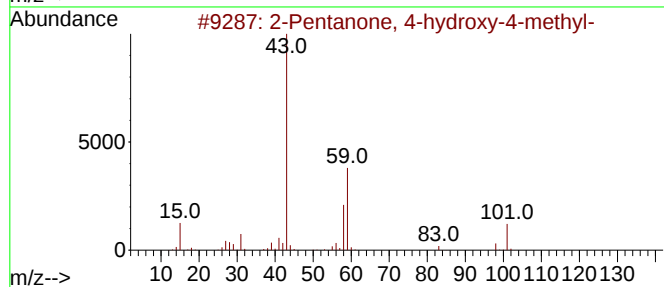
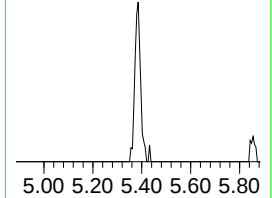
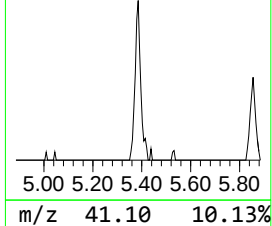
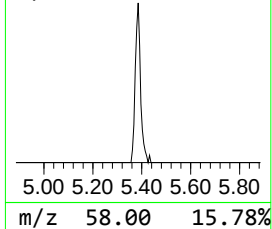
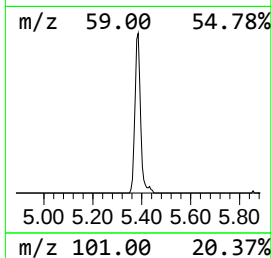
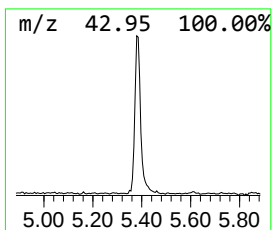
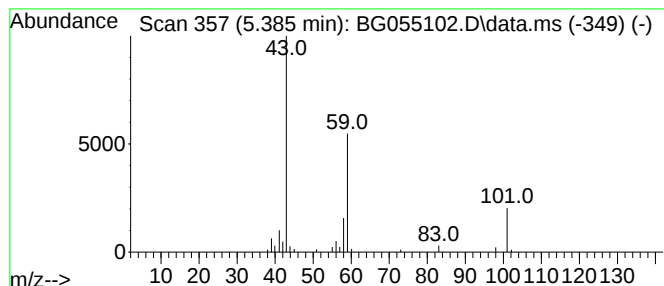
Instrument :
BNA_G
ClientSampleId :
DSN003

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.385	11.04 ng	79966	1,4-Dichlorobenzene-d4	8.334	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
5	Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9



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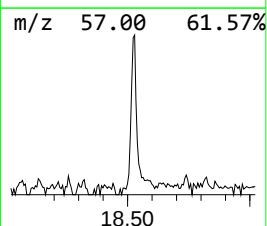
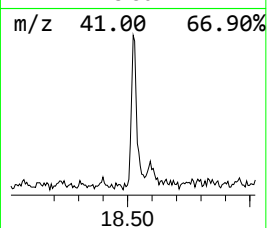
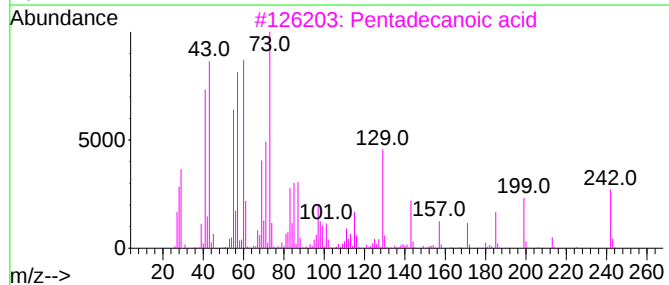
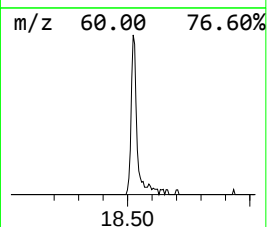
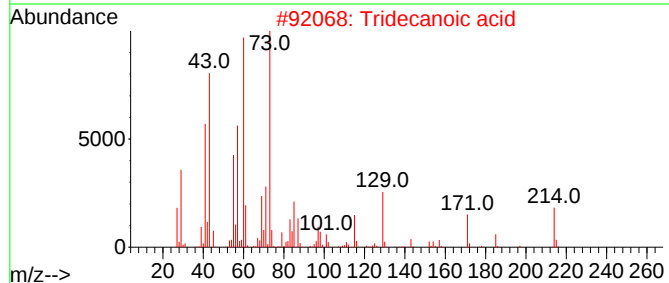
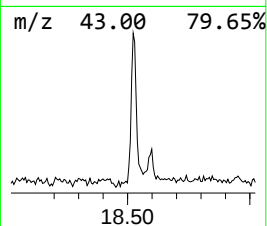
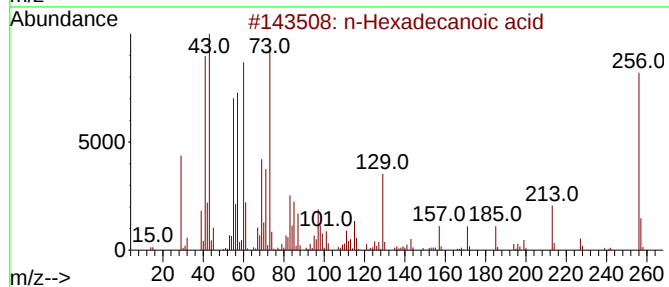
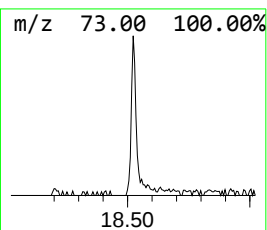
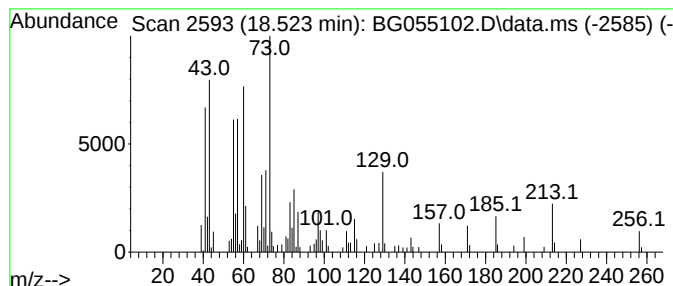
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.523	5.05 ng	115155	Phenanthrene-d10	17.671

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	47



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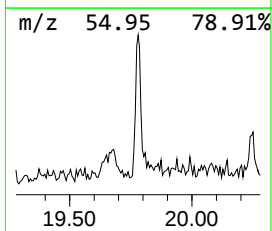
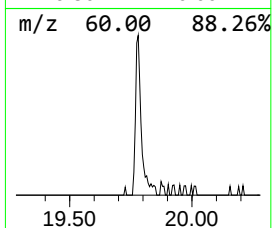
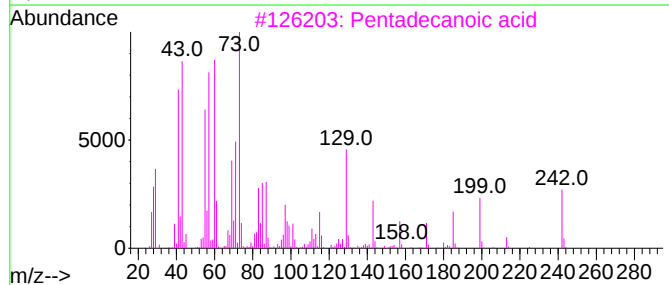
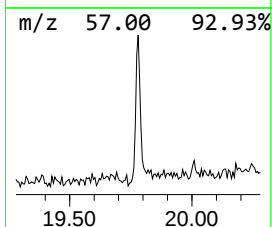
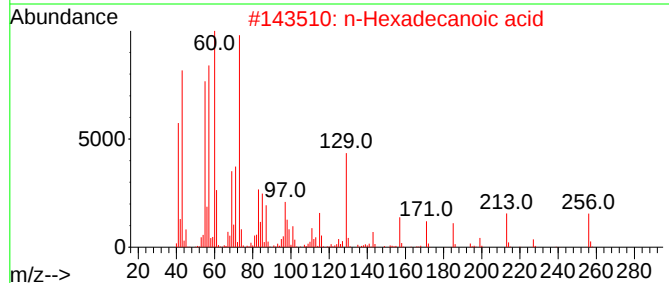
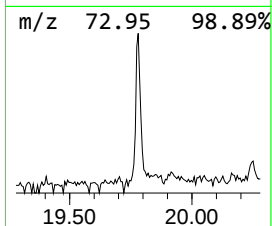
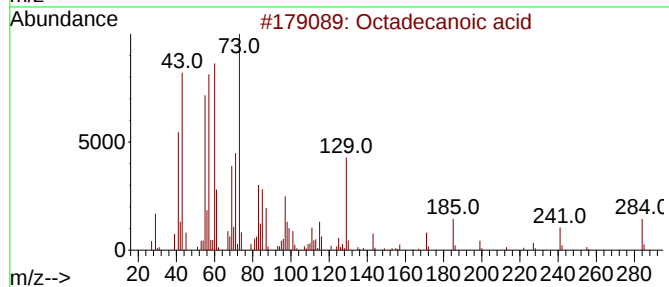
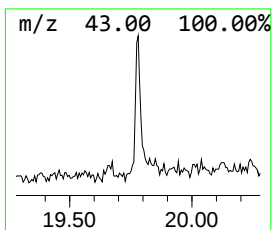
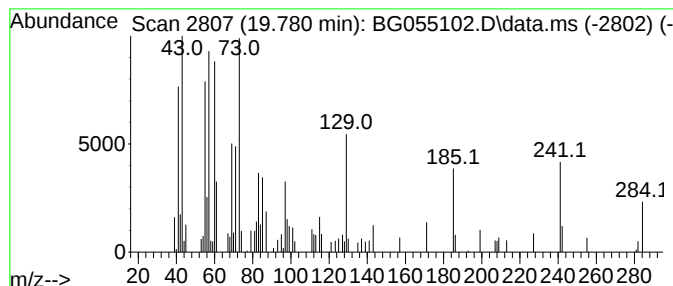
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.780	3.00 ng	68360	Phenanthrene-d10	17.671

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	81
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5			Undecanoic acid	186	C11H22O2	000112-37-8	55



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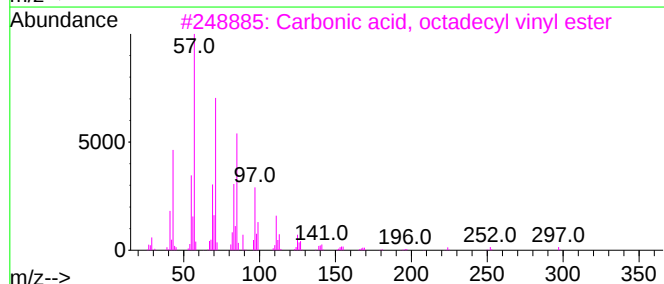
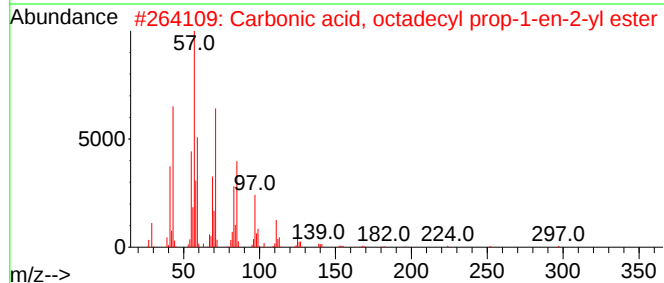
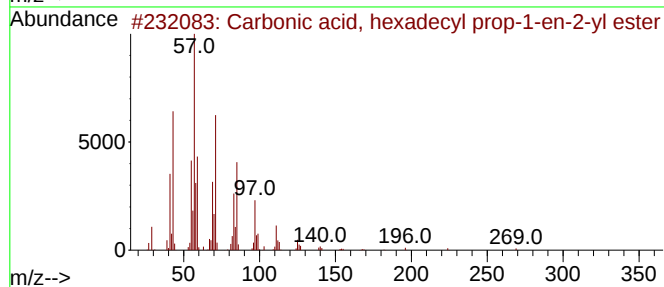
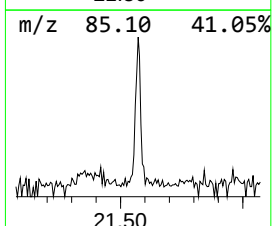
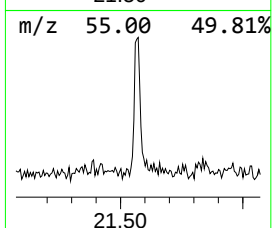
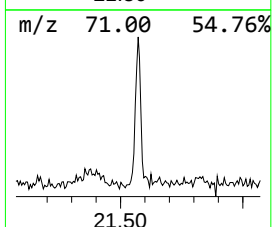
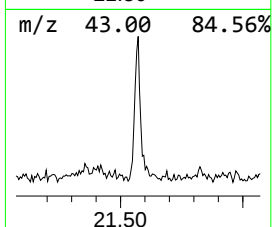
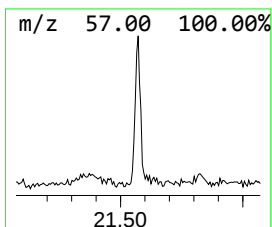
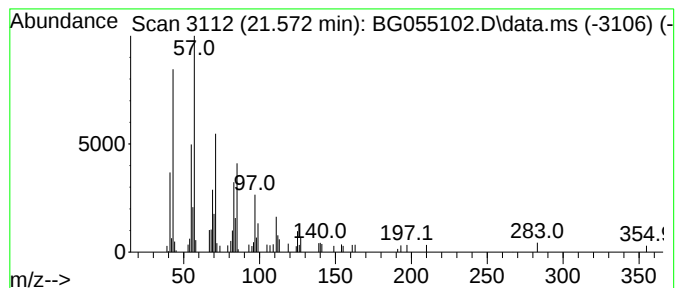
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Carbonic acid, hexadecyl pr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.572	2.61 ng	69694	Chrysene-d12	21.966

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
2			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
3			Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	90
4			Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	90
5			Isobutyl octadecyl ether	326	C22H46O	1000406-32-9	87



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.376	138.1	ng	1000560	1	8.334	144904	20.0
2-Pentanone, 4-...	5.385	11.0	ng	79966	1	8.334	144904	20.0
n-Hexadecanoic ...	18.523	5.0	ng	115155	4	17.671	455633	20.0
Octadecanoic acid	19.780	3.0	ng	68360	4	17.671	455633	20.0
Carbonic acid, ...	21.572	2.6	ng	69694	5	21.966	533496	20.0