

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121922\
 Data File : BG056020.D
 Acq On : 19 Dec 2022 19:30
 Operator : CG/JU
 Sample : N6065-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-S

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-BG121322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056020.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.399	15	19	30	rBB2	17891	27921	3.82%	0.843%
2	5.415	356	362	367	rBB2	15433	22973	3.15%	0.694%
3	5.885	436	442	449	rBB	123264	197153	26.99%	5.954%
4	7.500	709	717	724	rBB	125805	217016	29.71%	6.553%
5	8.370	859	865	871	rBB2	33208	53965	7.39%	1.630%
6	9.539	1057	1064	1071	rBB	78183	135026	18.49%	4.077%
7	11.202	1340	1347	1354	rBB	43880	75611	10.35%	2.283%
8	13.605	1749	1756	1763	rBB	262906	393256	53.84%	11.875%
9	14.974	1983	1989	1995	rBB	81062	125787	17.22%	3.798%
10	16.314	2212	2217	2221	rBV	6221	8539	1.17%	0.258%
11	16.449	2233	2240	2249	rVB	307956	456939	62.56%	13.799%
12	17.712	2447	2455	2460	rBV	115028	172547	23.62%	5.211%
13	18.558	2594	2599	2607	rBV2	34105	46345	6.34%	1.400%
14	19.475	2751	2755	2761	rVB4	5235	7880	1.08%	0.238%
15	19.739	2795	2800	2805	rBV	17879	23737	3.25%	0.717%
16	19.809	2806	2812	2821	rVB8	9677	16898	2.31%	0.510%
17	19.898	2823	2827	2829	rBV5	5283	8033	1.10%	0.243%
18	20.103	2857	2862	2869	rVB	25291	37744	5.17%	1.140%
19	20.285	2887	2893	2898	rBV	573377	730453	100.00%	22.058%
20	21.602	3114	3117	3124	rVB5	29382	44940	6.15%	1.357%
21	22.019	3179	3188	3194	rBV	129498	239056	32.73%	7.219%
22	22.876	3330	3334	3336	rBV5	7849	11934	1.63%	0.360%
23	23.828	3492	3496	3502	rVB7	13450	24535	3.36%	0.741%
24	25.515	3774	3783	3793	rBV2	75642	225296	30.84%	6.803%
25	27.442	4107	4111	4113	rBV4	5523	7913	1.08%	0.239%

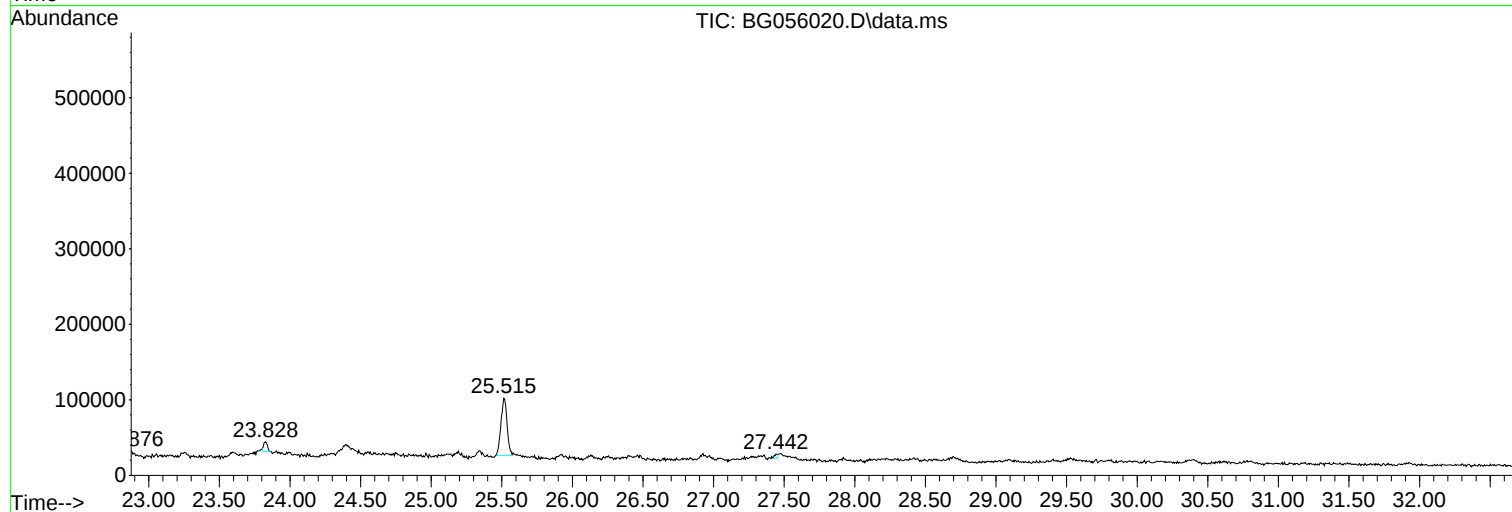
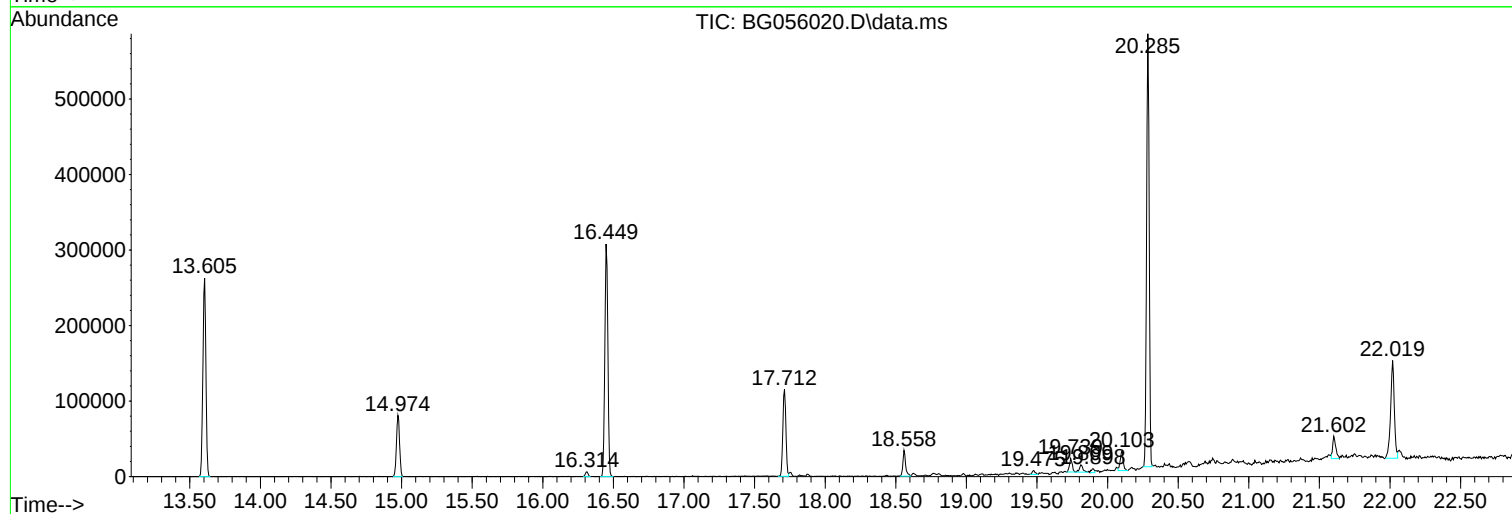
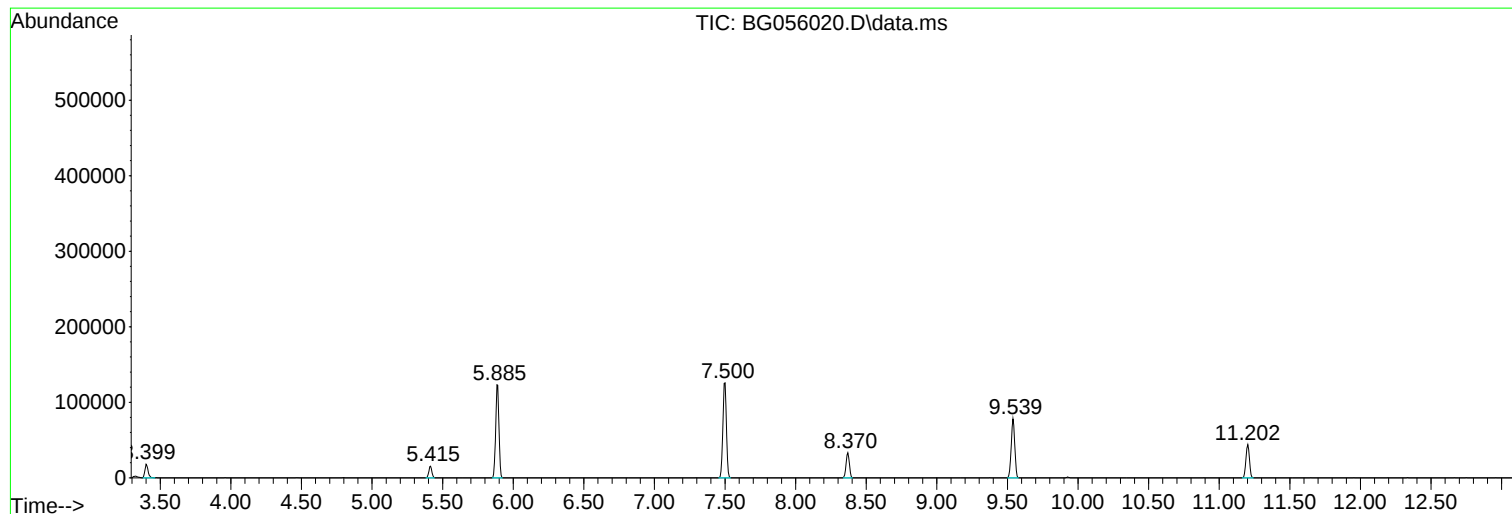
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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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Operator : CG/JU
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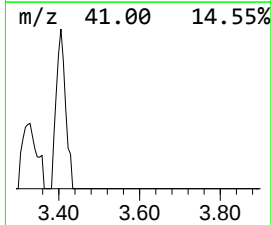
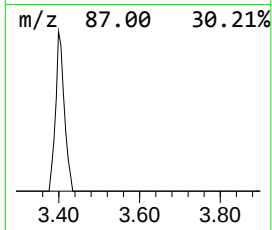
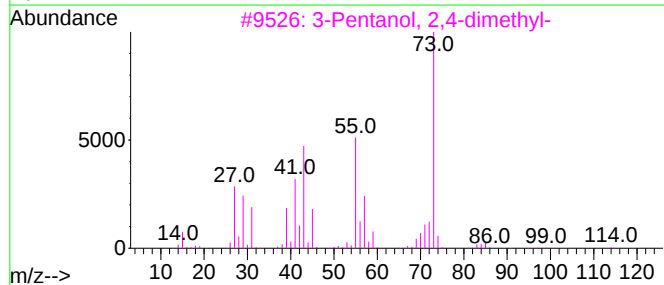
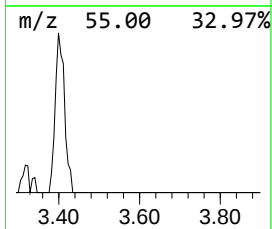
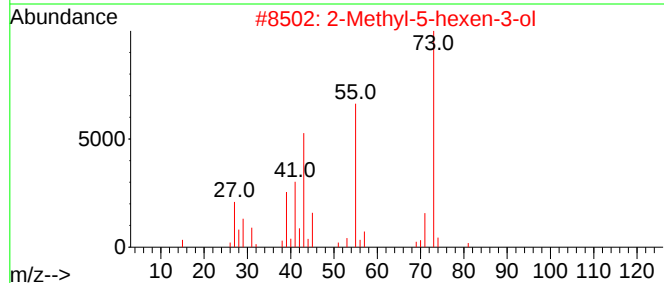
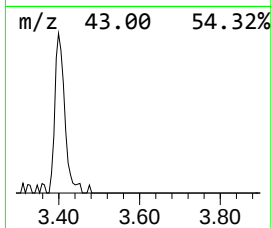
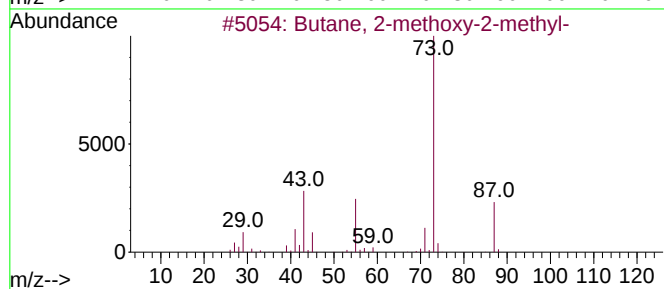
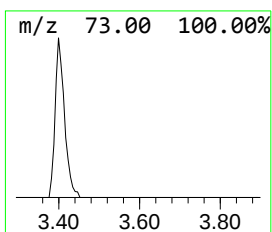
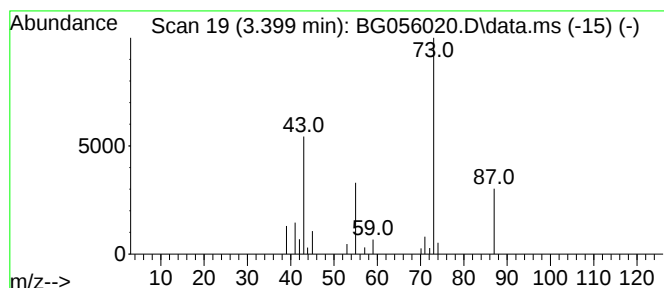
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.399	10.35 ng	27921	1,4-Dichlorobenzene-d4	8.370

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	53
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	17
4			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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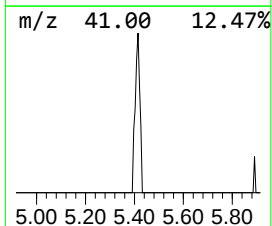
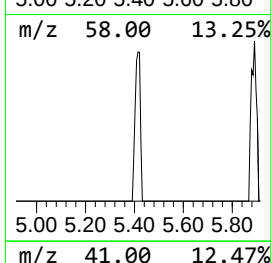
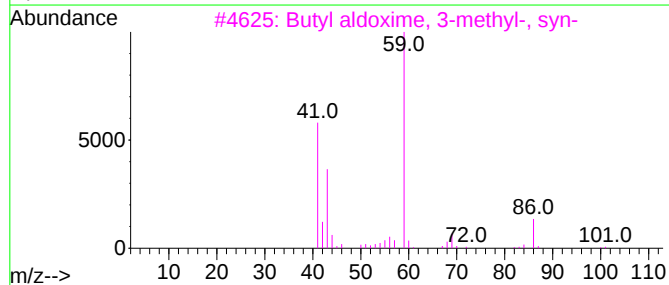
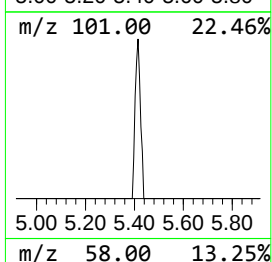
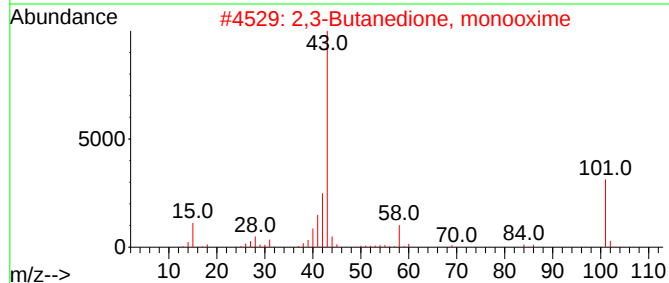
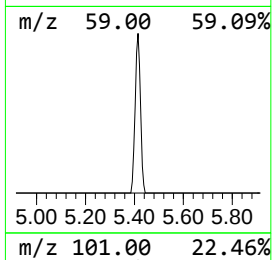
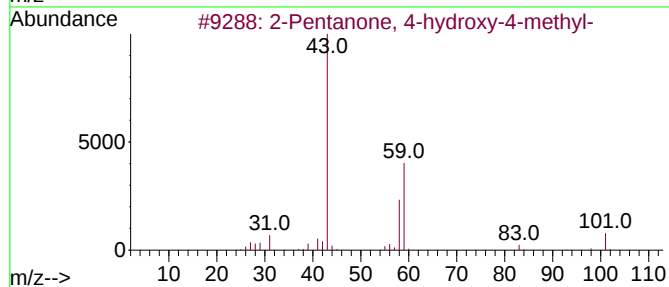
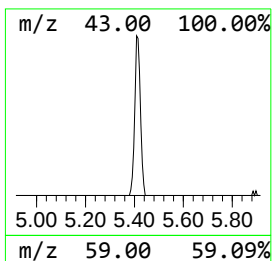
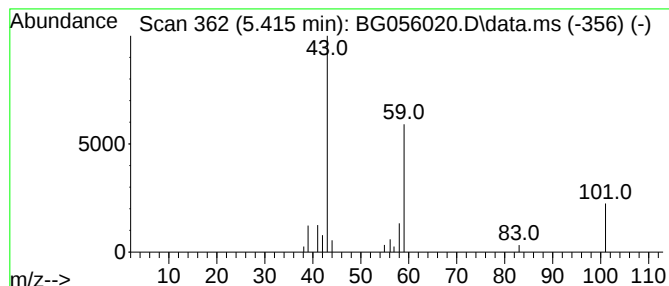
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.415	8.51 ng	22973	1,4-Dichlorobenzene-d4	8.370

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane	58	C4H10	000106-97-8	9



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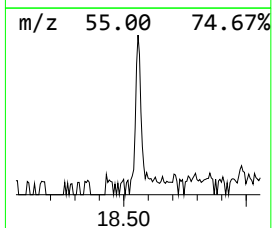
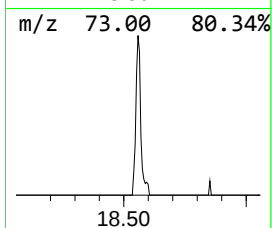
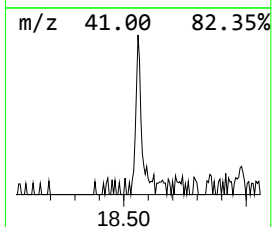
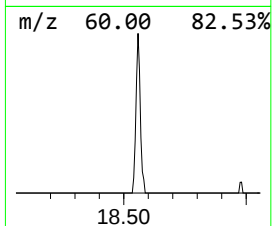
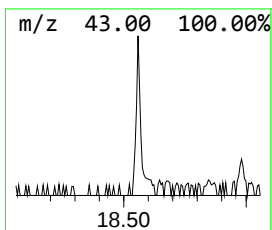
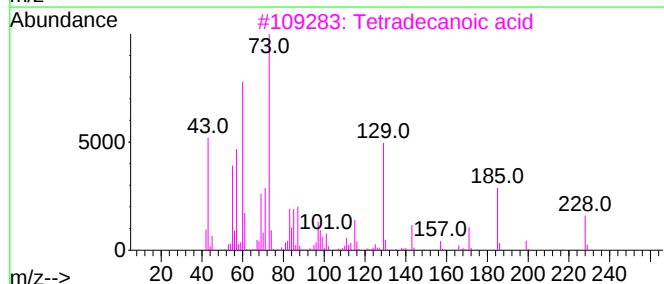
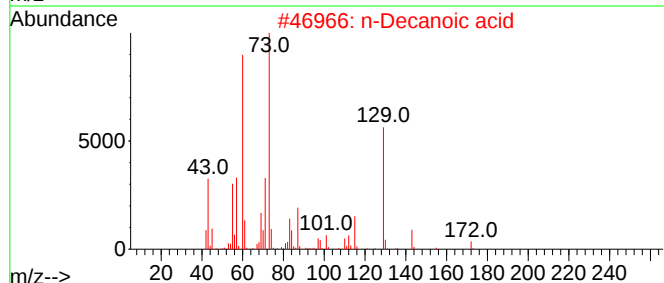
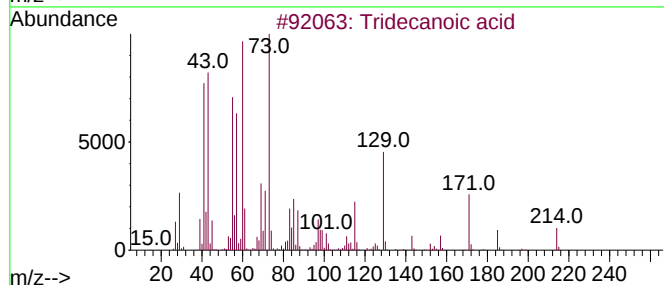
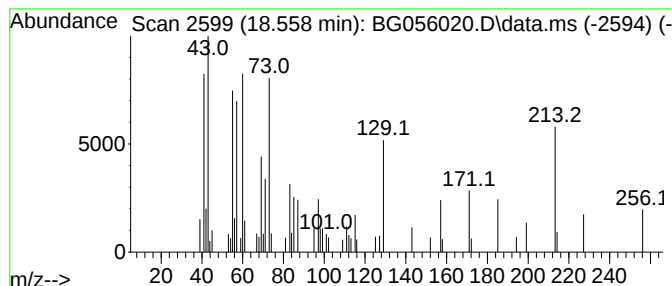
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.558	5.37 ng	46345	Phenanthrene-d10	17.712

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	92
2			n-Decanoic acid	172	C10H20O2	000334-48-5	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	43
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	38



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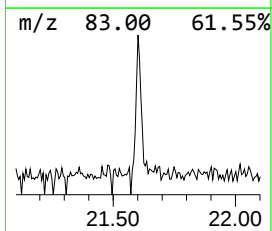
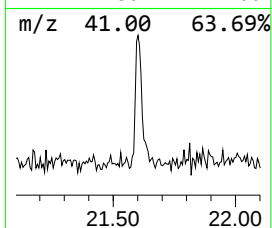
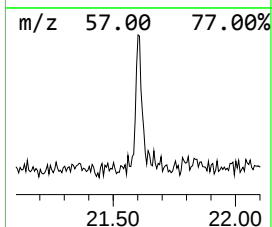
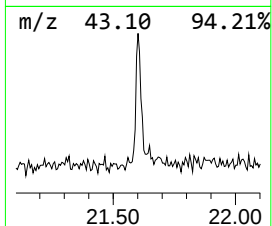
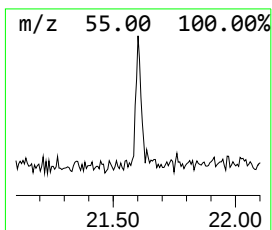
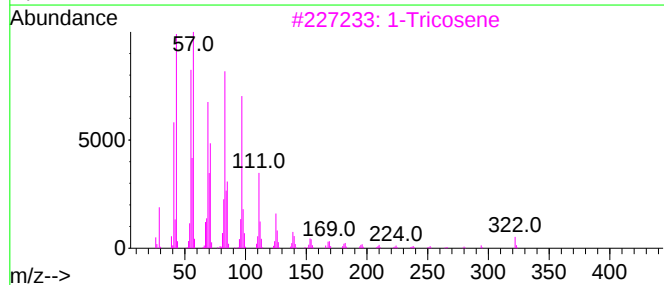
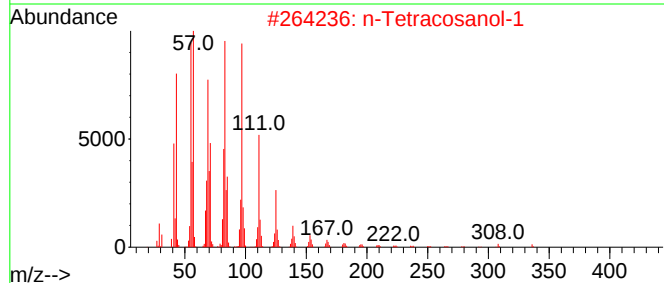
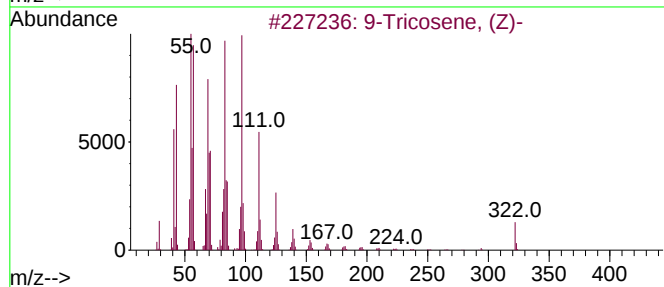
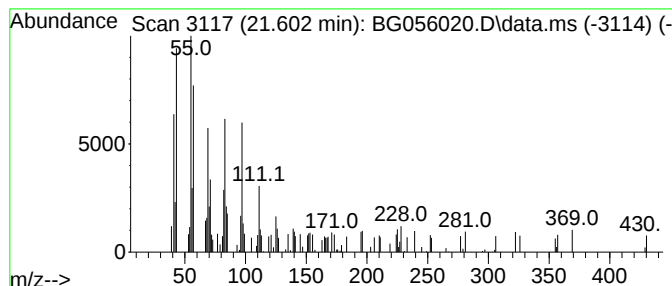
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9-Tricosene, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.602	3.76 ng	44940	Chrysene-d12	22.019

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3		1-Tricosene	322	C23H46	018835-32-0	90
4		1-Octadecene	252	C18H36	000112-88-9	86
5		Cyclotetradecane	196	C14H28	000295-17-0	83



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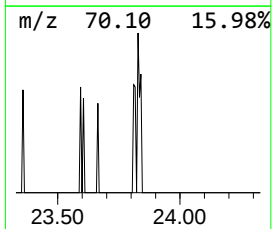
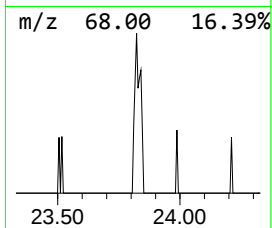
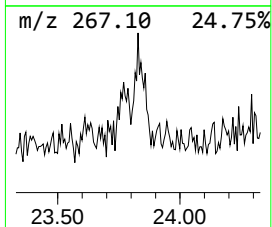
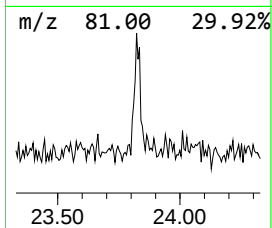
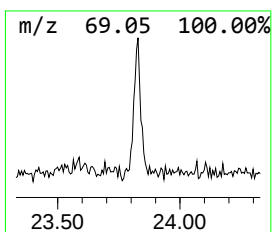
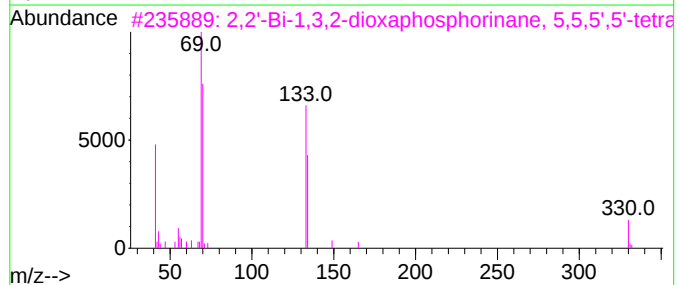
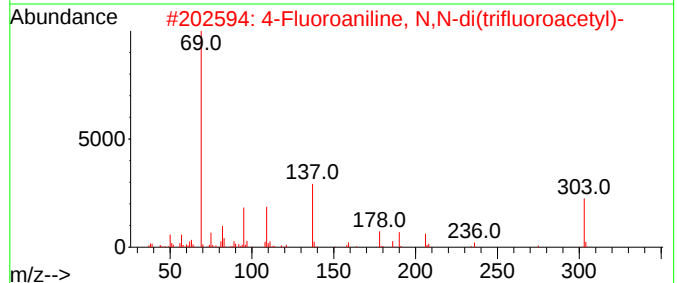
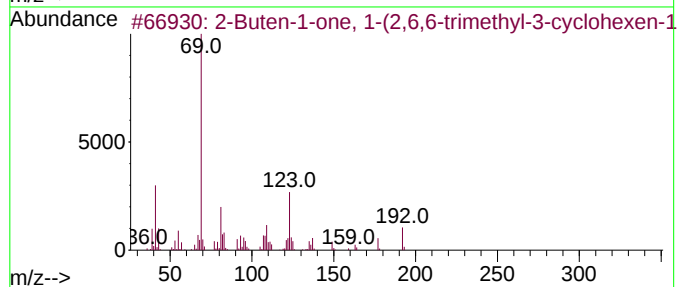
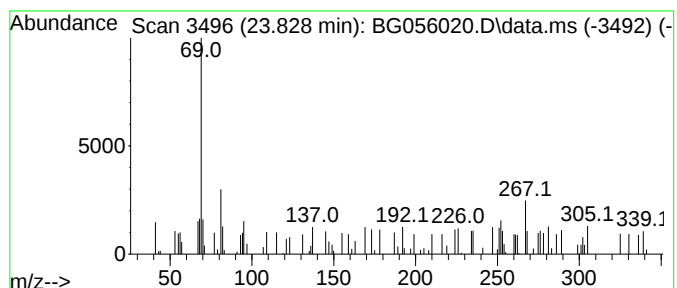
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown23.828 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.828	2.18 ng	24535	Perylene-d12	25.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Buten-1-one, 1-(2,6,6-trimethy...	192	C13H20O	041436-42-4	35		
2	4-Fluoroaniline, N,N-di(trifluor...	303	C10H4F7NO2	1000328-30-6	35		
3	2,2'-Bi-1,3,2-dioxaphosphorinane...	330	C10H20O4P2S2	016368-08-4	32		
4	Calcilactone B	422	C21H26O9	095349-43-2	25		
5	Cyclopentanecarboxamide, N-(4,5,...	330	C19H26N2O5	351061-05-7	23		



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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
Butane, 2-metho...	3.399	10.4	ng	27921	1	8.370	53965	20.0
2-Pentanone, 4-...	5.415	8.5	ng	22973	1	8.370	53965	20.0
Tridecanoic acid	18.558	5.4	ng	46345	4	17.712	172547	20.0
9-Tricosene, (Z)-	21.602	3.8	ng	44940	5	22.019	239056	20.0
unknown23.828	23.828	2.2	ng	24535	6	25.515	225296	20.0