

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122322\
 Data File : BG056086.D
 Acq On : 23 Dec 2022 19:55
 Operator : CG/JU
 Sample : N6072-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 LEFT-SIDE-SP-1215

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: BG056086.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.379	10	15	23	rBV	23907	36854	4.62%	1.061%
2	5.395	351	358	367	rVB	47868	72294	9.07%	2.081%
3	5.871	432	439	446	rBV	120764	190136	23.86%	5.474%
4	7.486	705	714	723	rVB	118823	206545	25.92%	5.947%
5	8.356	855	862	868	rBV	28694	47107	5.91%	1.356%
6	9.525	1054	1061	1068	rVB	75734	135110	16.95%	3.890%
7	11.188	1336	1344	1351	rBB	38733	67822	8.51%	1.953%
8	13.591	1746	1753	1760	rVB	248628	370481	46.49%	10.666%
9	14.966	1981	1987	1993	rVB	74934	117303	14.72%	3.377%
10	16.441	2232	2238	2246	rBV	343646	520322	65.29%	14.981%
11	17.698	2444	2452	2459	rBV	123283	183015	22.96%	5.269%
12	18.550	2592	2597	2607	rBV	29258	37862	4.75%	1.090%
13	19.801	2806	2810	2815	rBV4	7334	8434	1.06%	0.243%
14	20.277	2885	2891	2896	rBV	612997	796980	100.00%	22.946%
15	21.041	3014	3021	3027	rBV3	21090	32016	4.02%	0.922%
16	21.599	3111	3116	3126	rBV3	25473	48137	6.04%	1.386%
17	21.858	3156	3160	3164	rBV2	8709	12171	1.53%	0.350%
18	22.005	3178	3185	3192	rBV2	138818	234852	29.47%	6.762%
19	22.369	3242	3247	3251	rBV	12857	19960	2.50%	0.575%
20	23.244	3391	3396	3401	rVB4	9302	17290	2.17%	0.498%
21	23.732	3475	3479	3485	rVB9	4757	9825	1.23%	0.283%
22	25.495	3768	3779	3791	rVB2	84445	250813	31.47%	7.221%
23	26.893	4008	4017	4033	rBV6	14071	57997	7.28%	1.670%

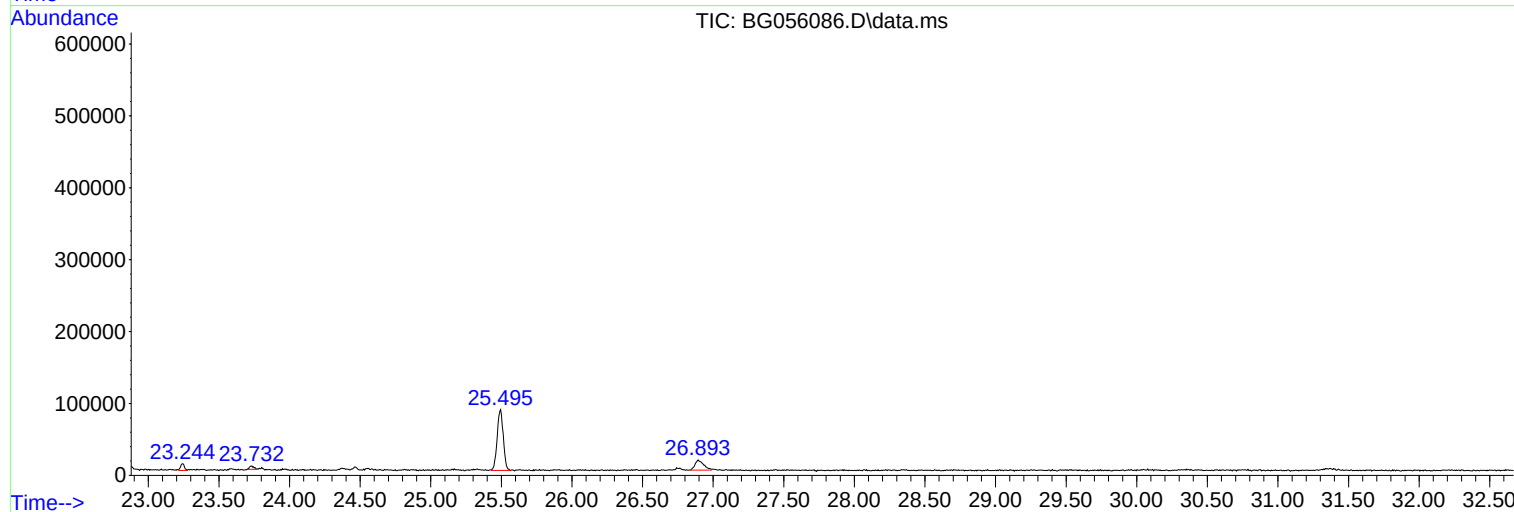
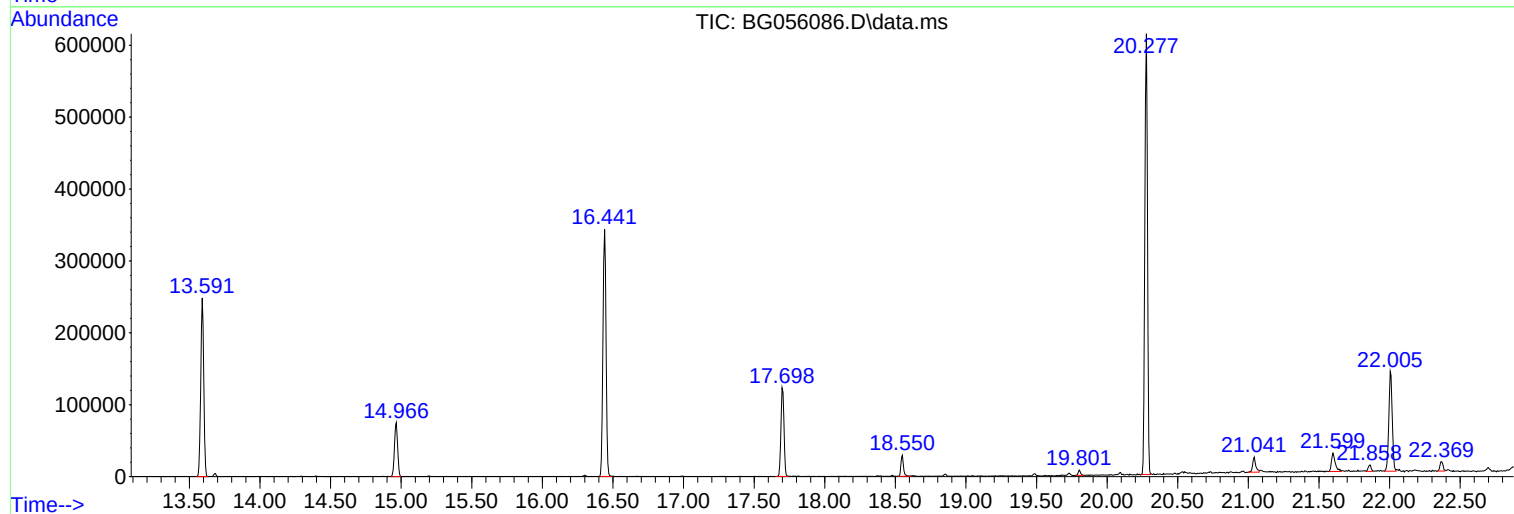
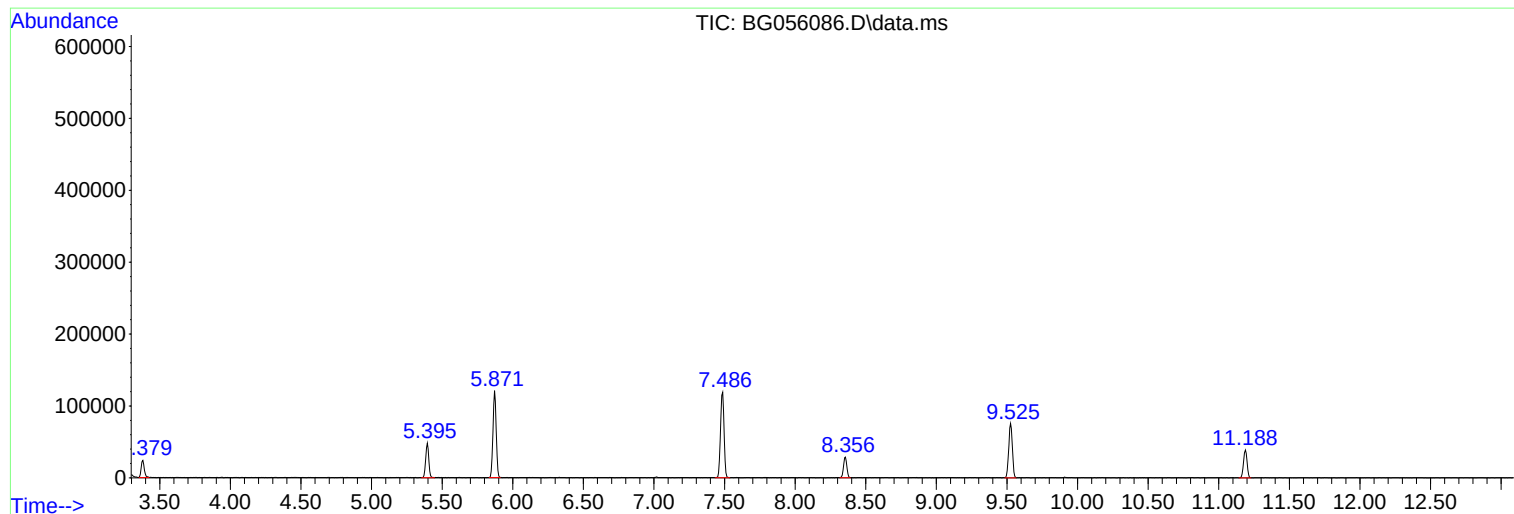
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LEFT-SIDE-SP-1215

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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Data File : BG056086.D
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Instrument :
BNA_G
ClientSampleId :
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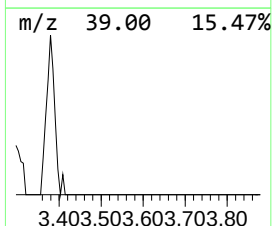
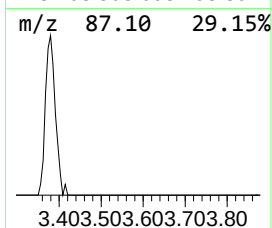
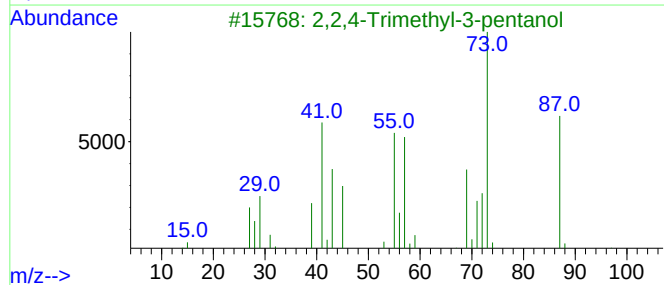
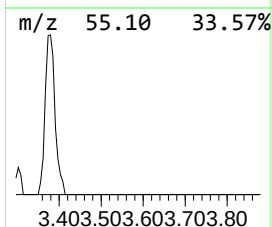
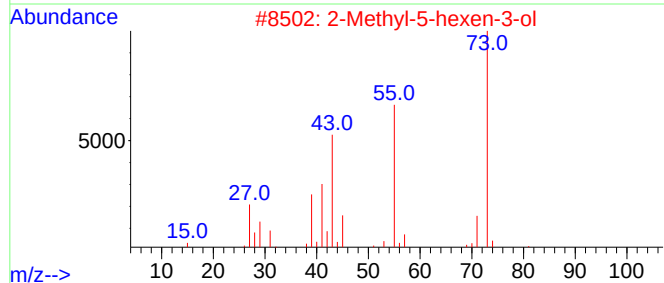
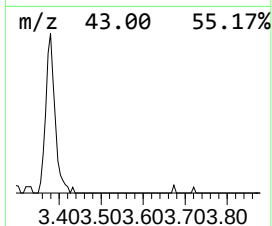
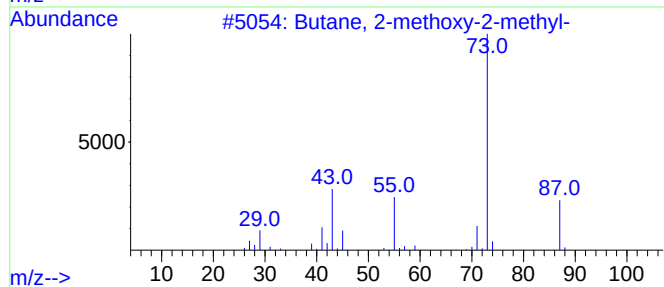
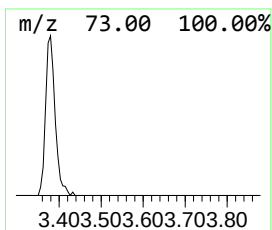
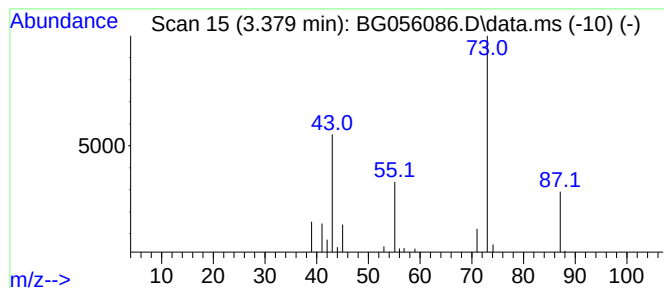
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.379	15.65 ng	36854	1,4-Dichlorobenzene-d4	8.356

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
4			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	33
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25



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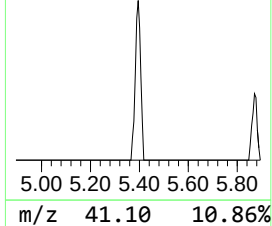
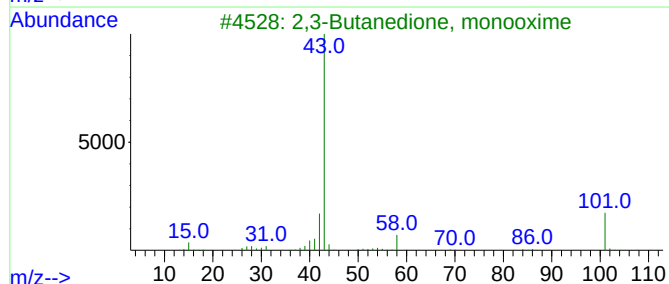
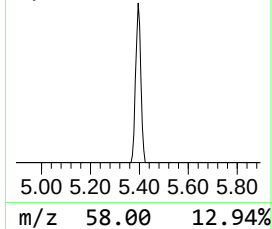
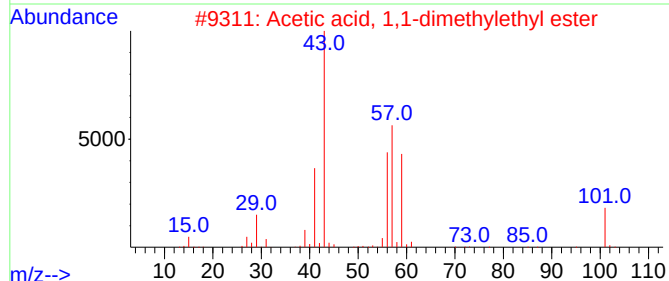
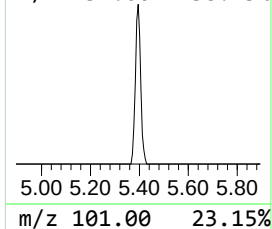
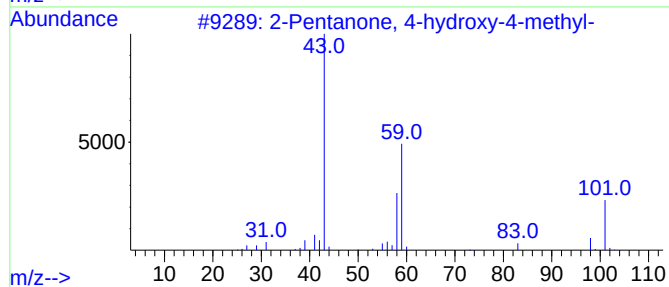
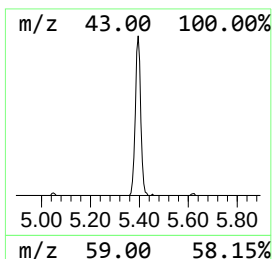
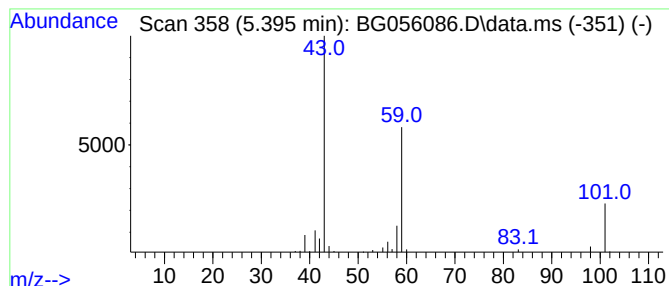
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.395	30.69 ng	72294	1,4-Dichlorobenzene-d4	8.356

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32
5			tert-Butyl Hydroperoxide	90	C4H10O2	000075-91-2	28



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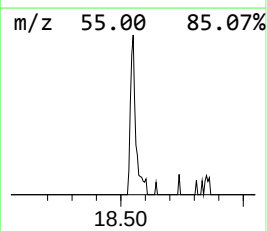
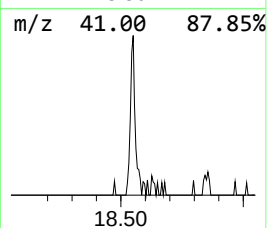
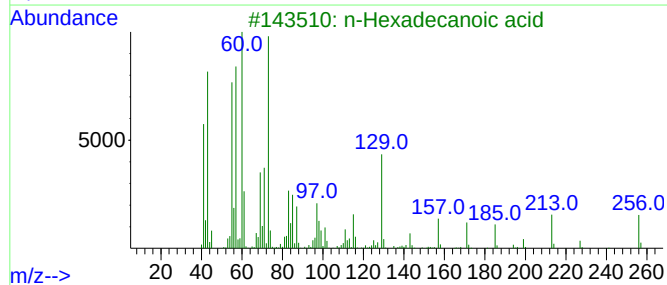
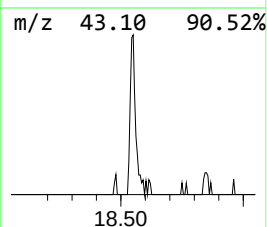
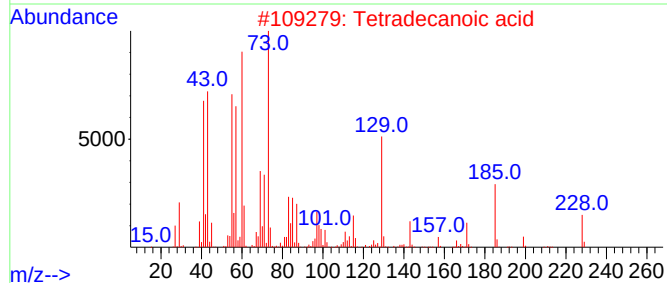
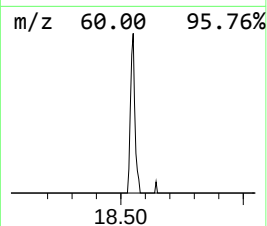
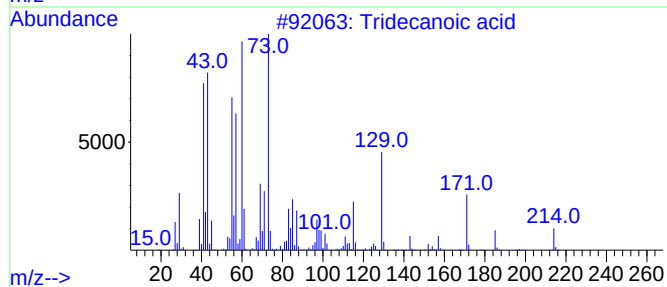
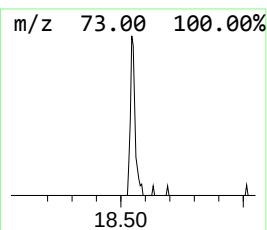
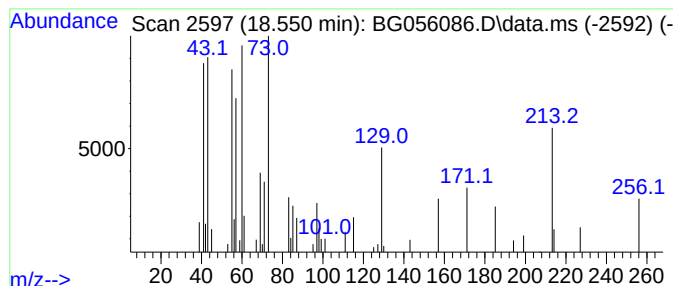
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.550	4.14 ng	37862	Phenanthrene-d10	17.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	96
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	49
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46
4			Dodecanoic acid	200	C12H24O2	000143-07-7	46
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	45



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Misc :
ALS Vial : 15 Sample Multiplier: 1

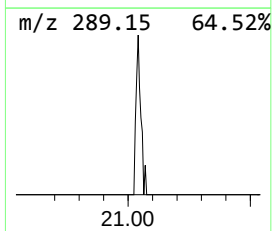
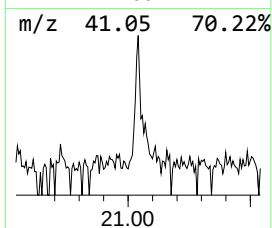
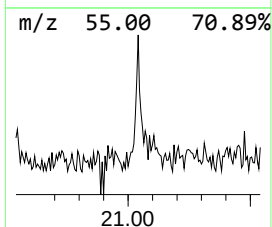
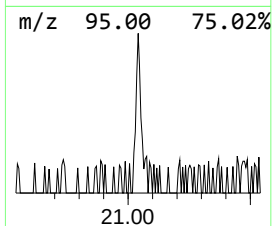
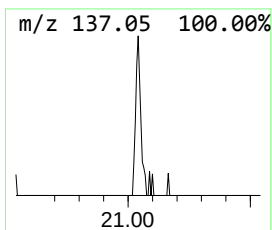
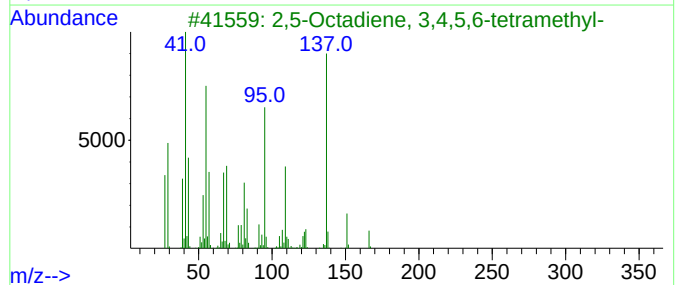
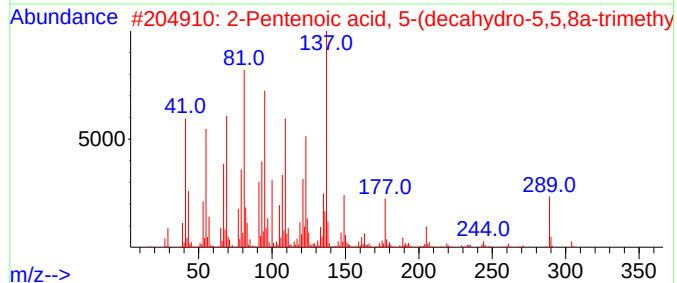
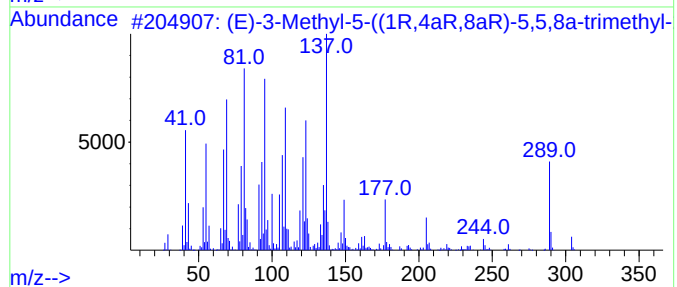
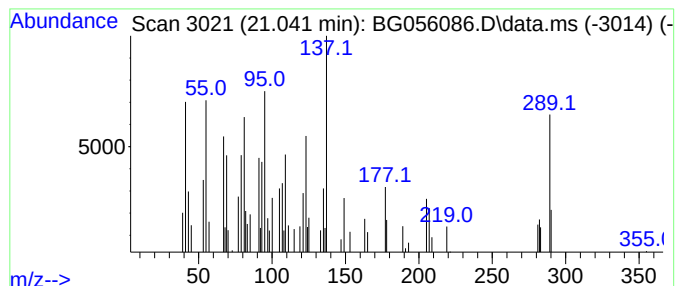
Instrument :
BNA_G
ClientSampleId :
LEFT-SIDE-SP-1215

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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 (E)-3-Methyl-5-((1R,4aR,8aR... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.041	2.73 ng	32016	Chrysene-d12	22.005	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Methyl-5-((1R,4aR,8aR)-5,5...	304	C20H32O2	020257-75-4	68
2	2-Pentenoic acid, 5-(decahydro-5...	304	C20H32O2	024470-48-2	62
3	2,5-Octadiene, 3,4,5,6-tetramethyl-	166	C12H22	247797-85-9	43
4	cis-4a-Methyl-decahydronaphthalene	152	C11H20	002547-26-4	38
5	Androstan-7-one, oxime, (5.alpha.)-	289	C19H31NO	054156-20-6	30



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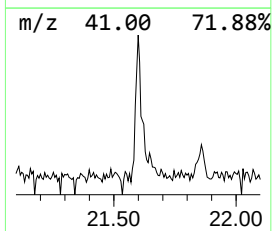
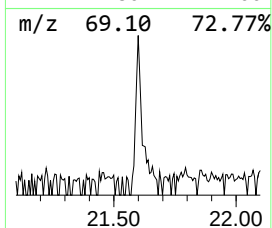
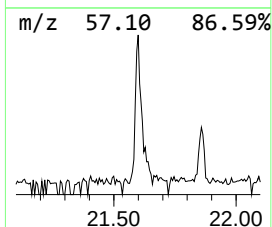
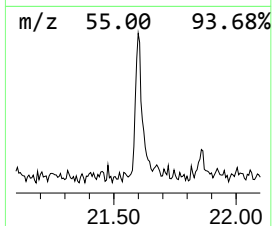
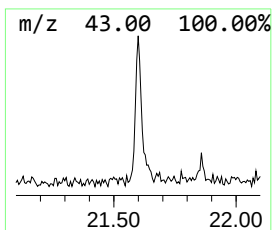
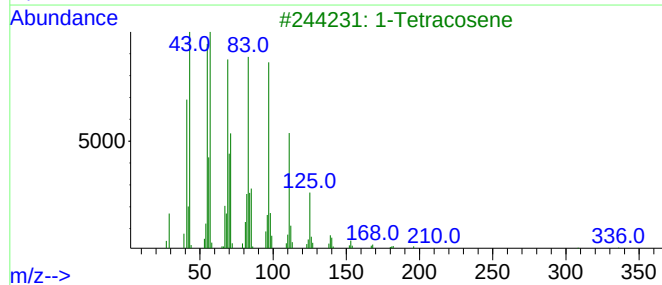
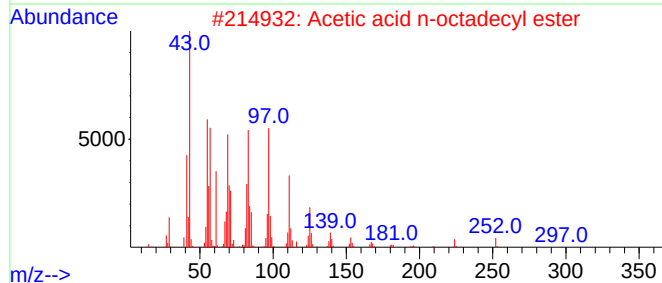
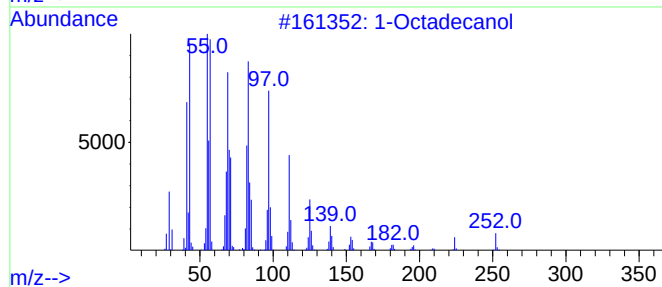
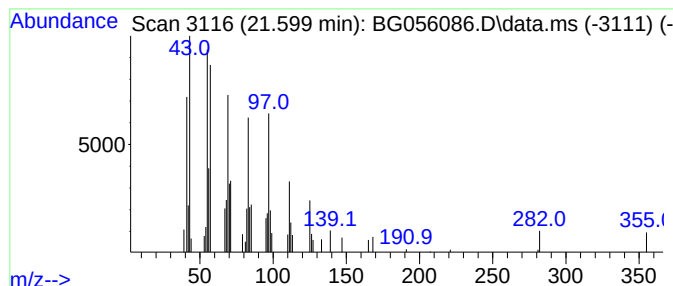
Instrument :
BNA_G
ClientSampleId :
LEFT-SIDE-SP-1215

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

Peak Number 5 1-Octadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.599	4.10 ng	48137	Chrysene-d12	22.005	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	91
2	Acetic acid n-octadecyl ester	312	C20H40O2	000822-23-1	90
3	1-Tetracosene	336	C24H48	010192-32-2	87
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
5	1-Tricosanol	340	C23H48O	003133-01-5	87



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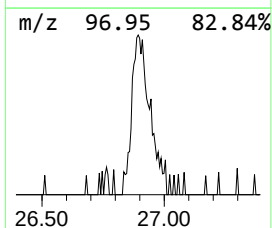
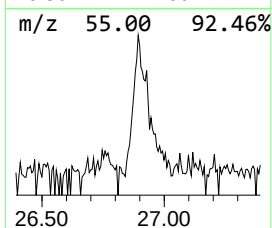
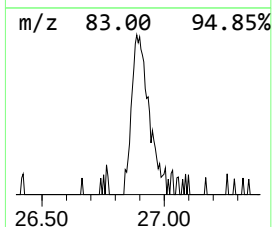
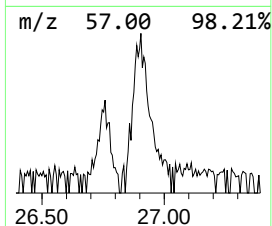
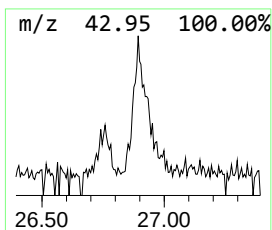
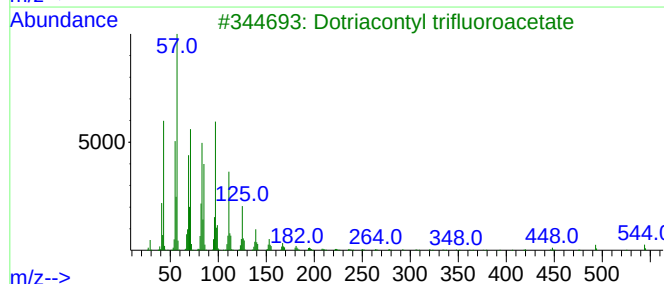
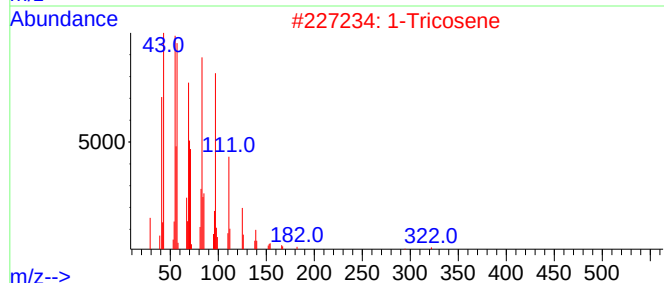
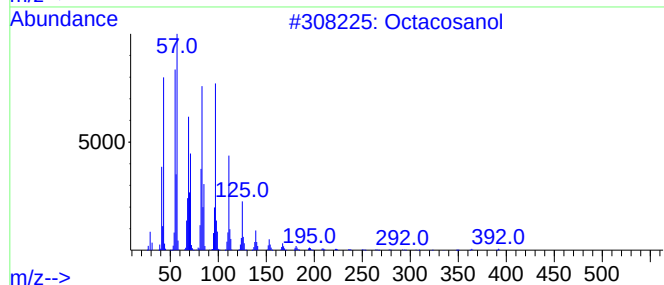
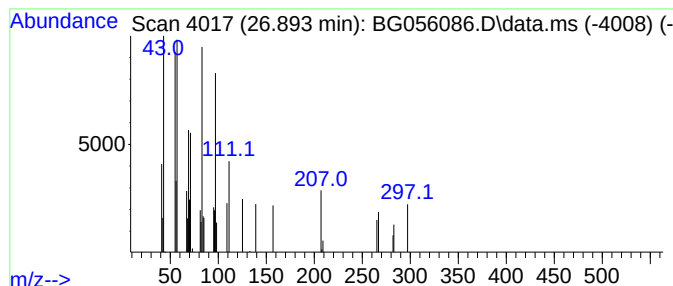
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.893	4.62 ng	57997	Perylene-d12	25.495

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanol	410	C28H58O	000557-61-9	58
2			1-Tricosene	322	C23H46	018835-32-0	58
3			Dotriacontyl trifluoroacetate	562	C34H65F3O2	1000351-75-4	46
4			Triacetyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	46
5			Tetratriacontyl trifluoroacetate	591	C36H69F3O2	1000351-75-3	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122322\
Data File : BG056086.D
Acq On : 23 Dec 2022 19:55
Operator : CG/JU
Sample : N6072-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LEFT-SIDE-SP-1215

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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
Butane, 2-metho...	3.379	15.7	ng	36854	1	8.356	47107	20.0
2-Pentanone, 4-...	5.395	30.7	ng	72294	1	8.356	47107	20.0
Tridecanoic acid	18.550	4.1	ng	37862	4	17.698	183015	20.0
(E)-3-Methyl-5-...	21.041	2.7	ng	32016	5	22.005	234852	20.0
1-Octadecanol	21.599	4.1	ng	48137	5	22.005	234852	20.0
Octacosanol	26.893	4.6	ng	57997	6	25.495	250813	20.0