

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
 Data File : BG048988.D
 Acq On : 15 Jun 2021 22:06
 Operator : CG/JU
 Sample : M2672-12
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 17-B6(52-56)

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-BG061121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048988.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.159	15	20	29	rVB3	143796	221422	11.94%	2.254%
2	3.283	37	41	47	rVB	51316	69954	3.77%	0.712%
3	5.198	362	367	374	rBV2	12917	23853	1.29%	0.243%
4	5.662	440	446	453	rBV	453629	755451	40.75%	7.691%
5	5.733	453	458	468	rVB2	15381	36123	1.95%	0.368%
6	7.266	711	719	728	rBV	448849	804245	43.38%	8.188%
7	8.112	855	863	869	rBV2	118854	209468	11.30%	2.133%
8	9.276	1054	1061	1074	rVB	270443	501281	27.04%	5.104%
9	10.703	1297	1304	1309	rBV	12739	23526	1.27%	0.240%
10	10.938	1337	1344	1351	rBV	147959	270750	14.60%	2.756%
11	13.377	1752	1759	1766	rBV	677647	1049503	56.61%	10.685%
12	14.757	1985	1994	2002	rBV	247072	399516	21.55%	4.067%
13	16.156	2225	2232	2237	rBV	34265	47071	2.54%	0.479%
14	16.244	2240	2247	2255	rBV	640097	977888	52.75%	9.956%
15	17.501	2452	2461	2469	rBV	355798	562648	30.35%	5.728%
16	17.619	2477	2481	2486	rVB4	38083	52103	2.81%	0.530%
17	18.159	2568	2573	2581	rVB5	24129	36356	1.96%	0.370%
18	18.388	2607	2612	2619	rBV2	83595	129775	7.00%	1.321%
19	19.657	2823	2828	2835	rBV2	60646	83900	4.53%	0.854%
20	20.110	2899	2905	2911	rBV	1407408	1853849	100.00%	18.874%
21	20.797	3015	3022	3025	rBV6	21789	42241	2.28%	0.430%
22	20.868	3031	3034	3038	rVB3	19143	21843	1.18%	0.222%
23	21.426	3124	3129	3138	rBV2	97472	162296	8.75%	1.652%
24	21.684	3168	3173	3177	rVB	40516	55330	2.98%	0.563%
25	21.796	3185	3192	3202	rVB2	390081	665020	35.87%	6.771%
26	22.002	3224	3227	3231	rVB5	14403	20434	1.10%	0.208%
27	22.642	3331	3336	3342	rBV7	15549	28950	1.56%	0.295%
28	23.018	3396	3400	3406	rVB7	27170	45498	2.45%	0.463%
29	25.128	3749	3759	3770	rBV2	217139	671945	36.25%	6.841%

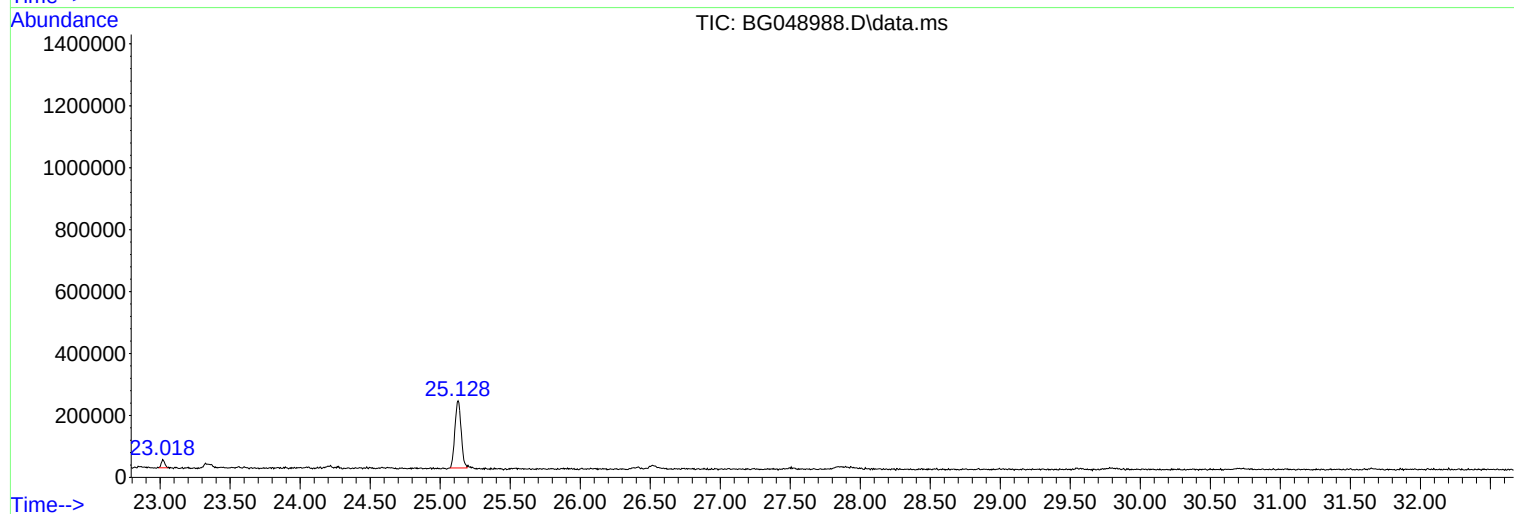
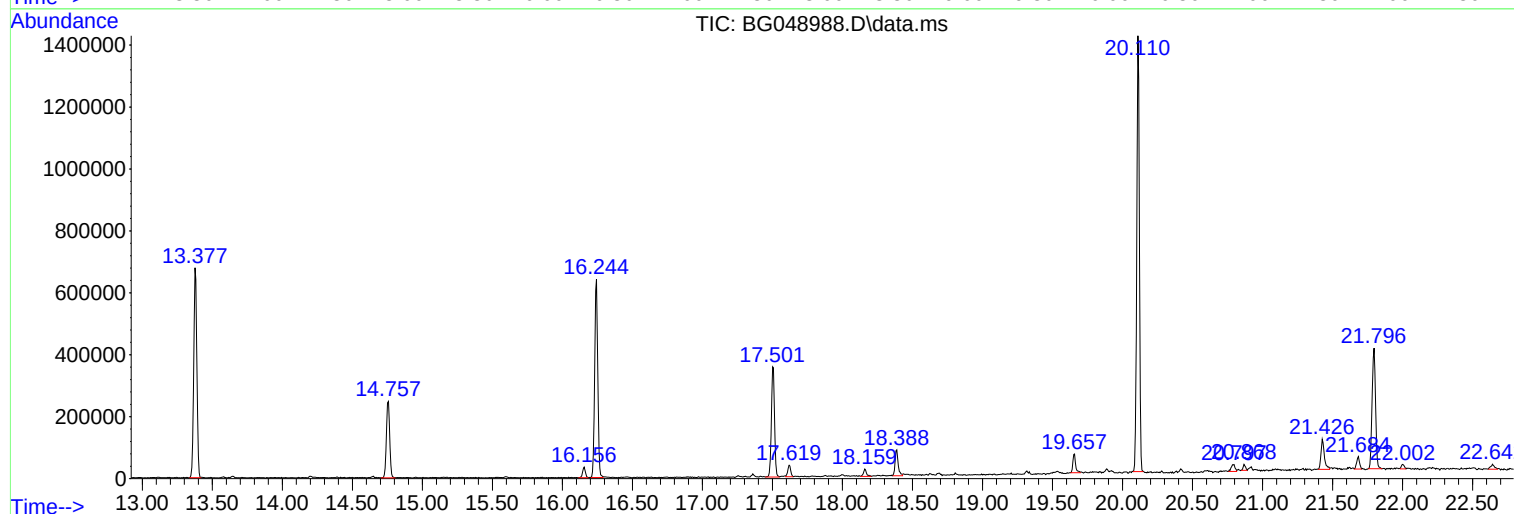
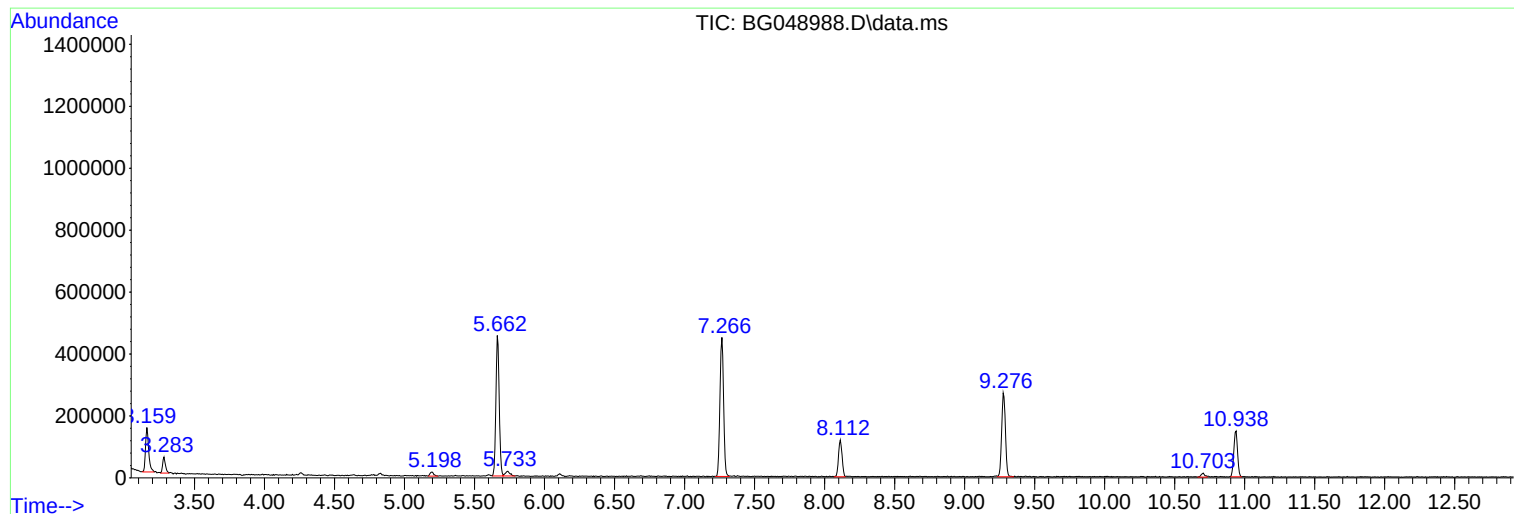
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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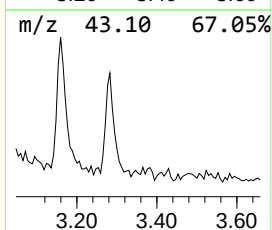
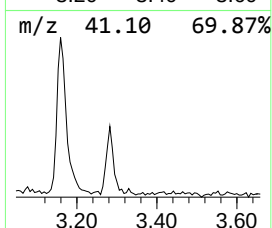
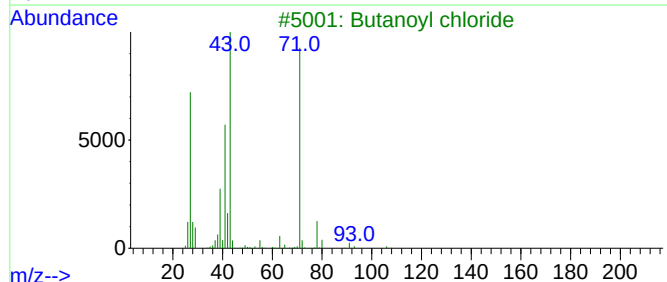
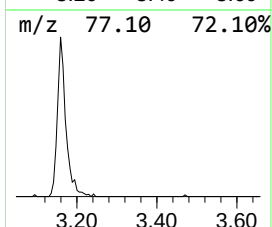
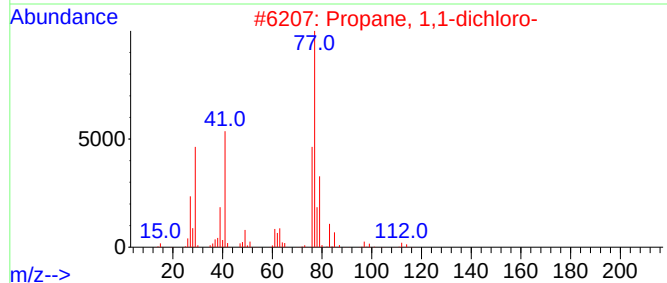
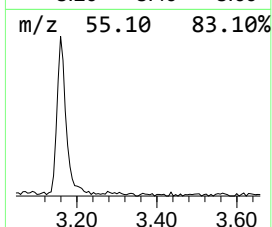
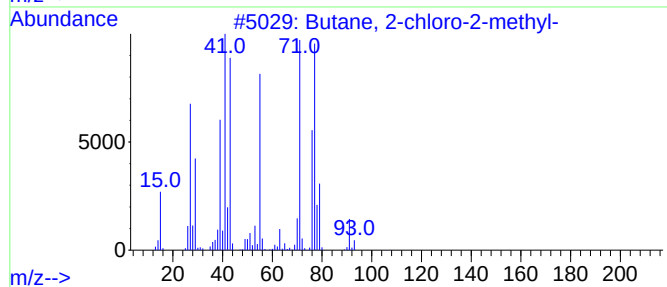
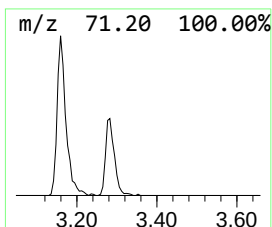
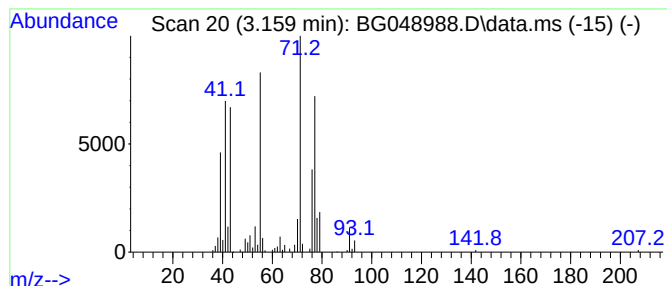
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.159	21.14 ng	221422	1,4-Dichlorobenzene-d4	8.112

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	90
2			Propane, 1,1-dichloro-	112	C3H6Cl2	000078-99-9	27
3			Butanoyl chloride	106	C4H7ClO	000141-75-3	27
4			Allyl chloride	76	C3H5Cl	000107-05-1	22
5			Furan-2-carbonyl chloride, tetra...	134	C5H7ClO2	052449-98-6	14



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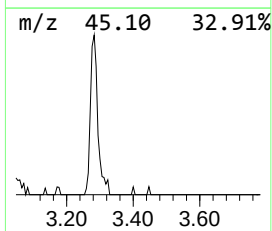
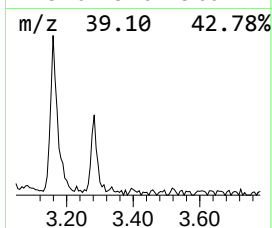
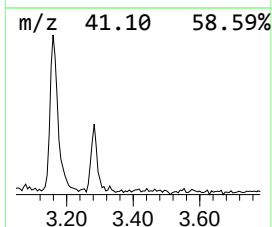
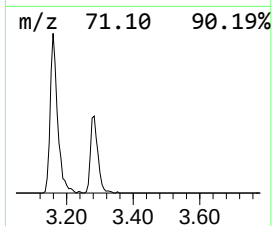
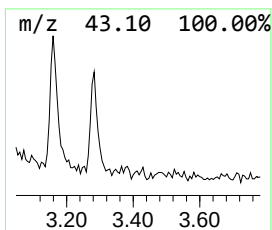
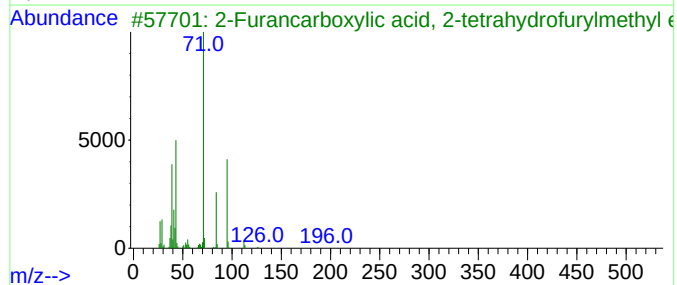
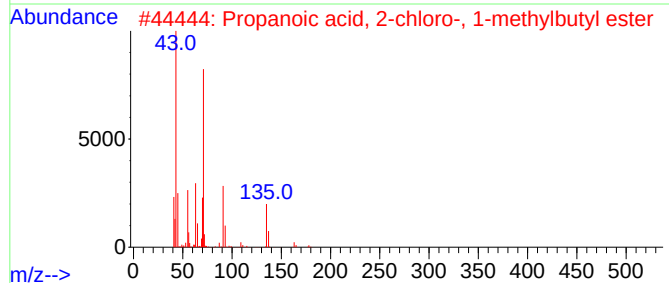
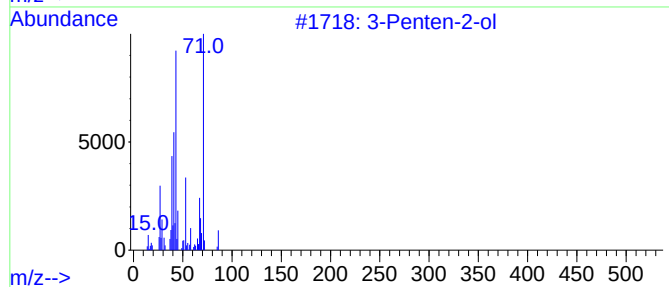
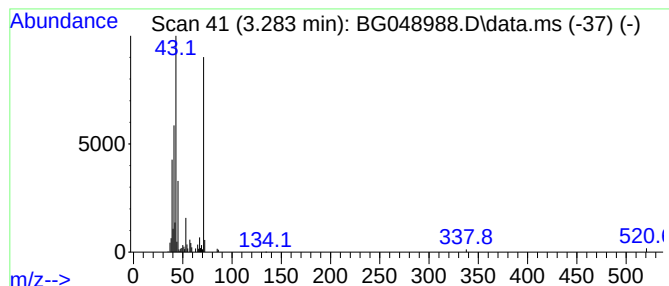
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-ol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.283	6.68 ng	69954	1,4-Dichlorobenzene-d4	8.112

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-ol	86	C5H10O	001569-50-2	72
2			Propanoic acid, 2-chloro-, 1-met...	178	C8H15ClO2	088736-64-5	72
3			2-Furancarboxylic acid, 2-tetrahydrofurylmethyl ester	196	C10H12O4	004623-04-5	45
4			2-Oxo-n-valeric acid	116	C5H8O3	001821-02-9	43
5			Pentane, 2,2'-oxybis-	158	C10H22O	056762-00-6	40



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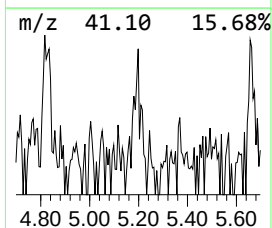
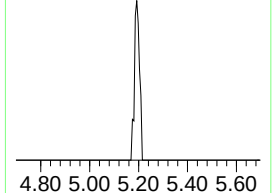
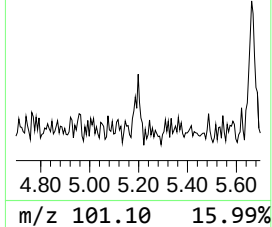
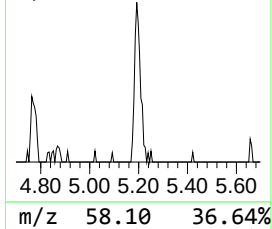
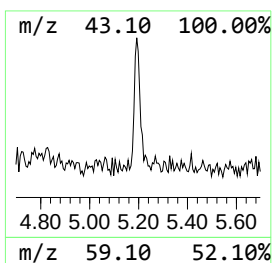
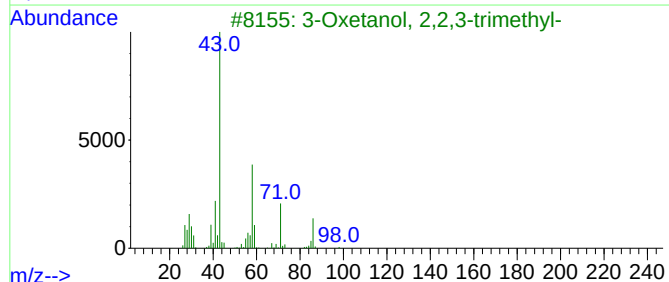
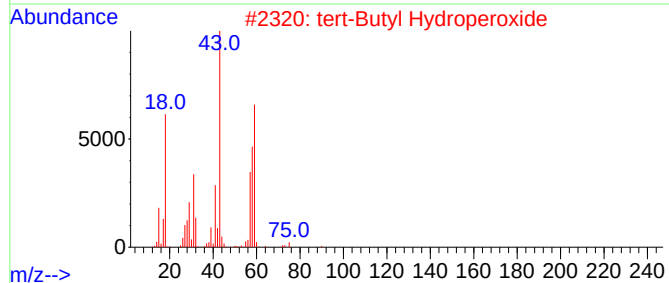
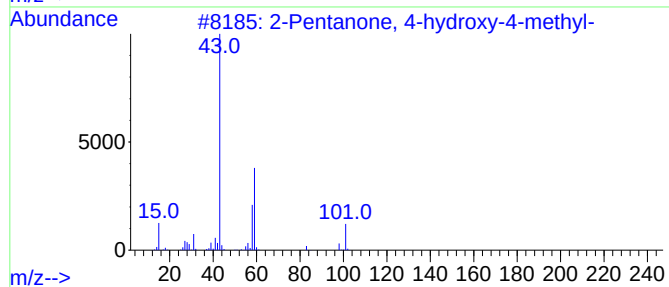
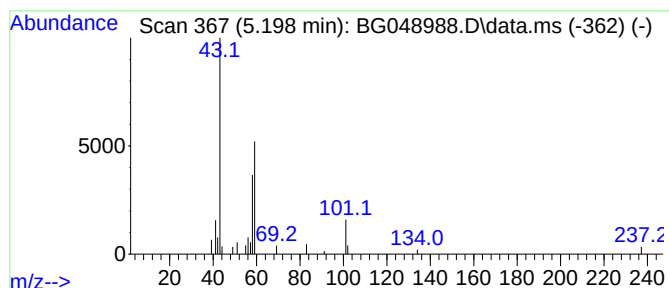
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.198	2.28 ng	23853	1,4-Dichlorobenzene-d4	8.112

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			tert-Butyl Hydroperoxide	90	C4H10O2	000075-91-2	36
3			3-Oxetanol, 2,2,3-trimethyl-	116	C6H12O2	025910-96-7	17
4			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	9
5			Acetone	58	C3H6O	000067-64-1	9



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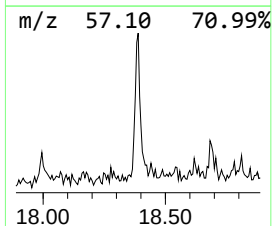
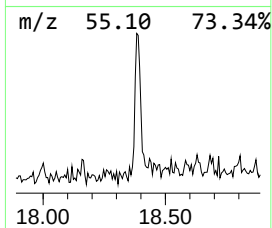
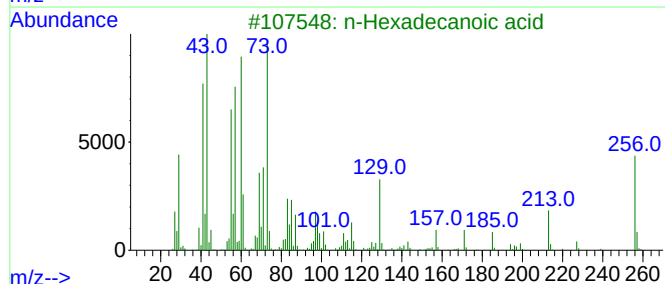
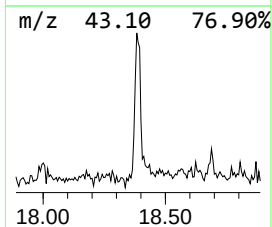
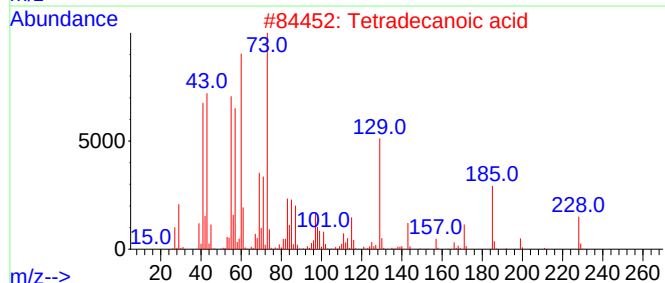
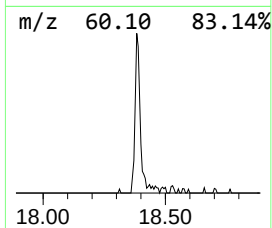
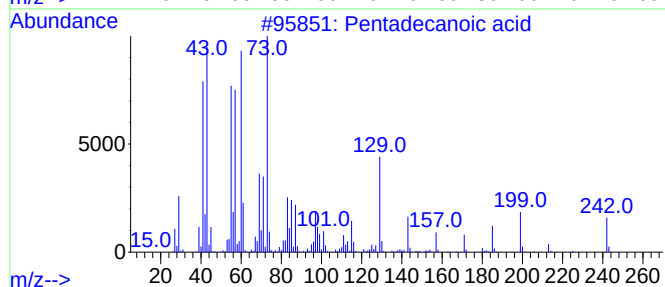
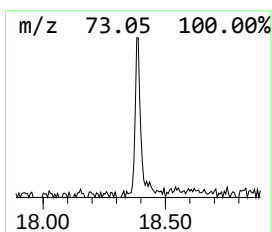
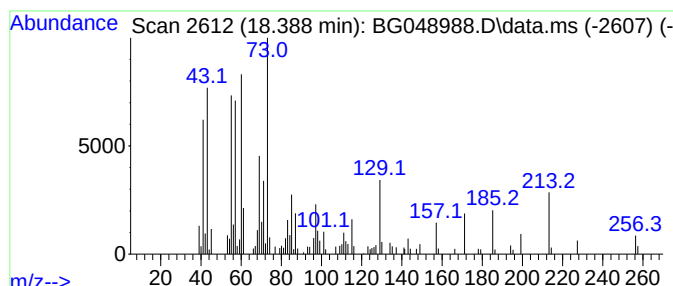
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.388	4.61 ng	129775	Phenanthrene-d10	17.501

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
4			Tridecanoic acid	214	C13H26O2	000638-53-9	53
5			Dodecanoic acid	200	C12H24O2	000143-07-7	52



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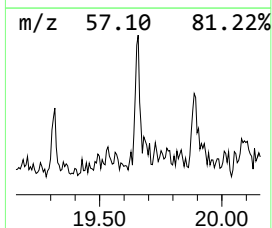
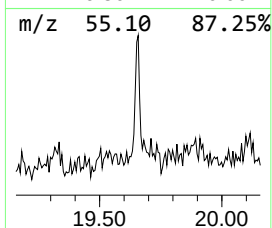
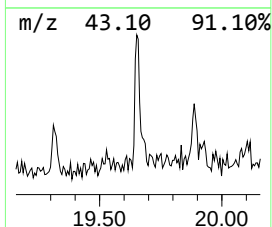
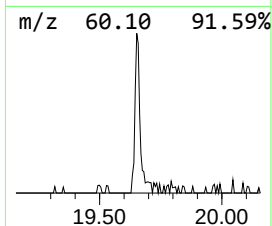
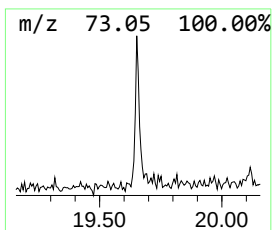
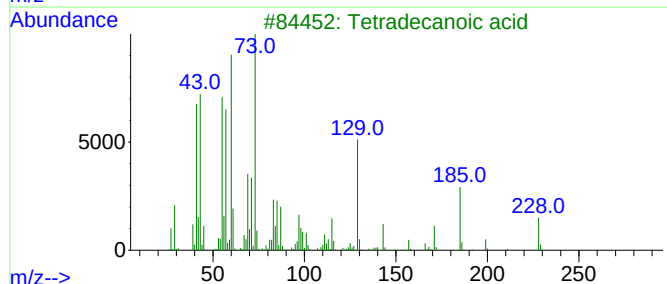
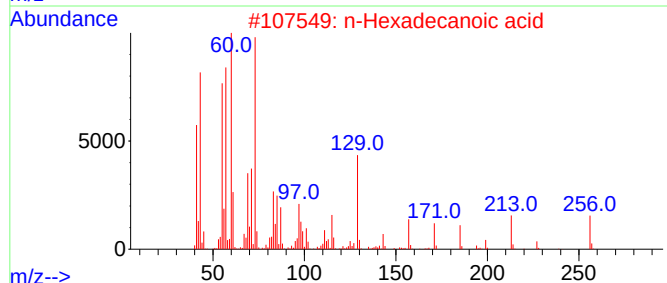
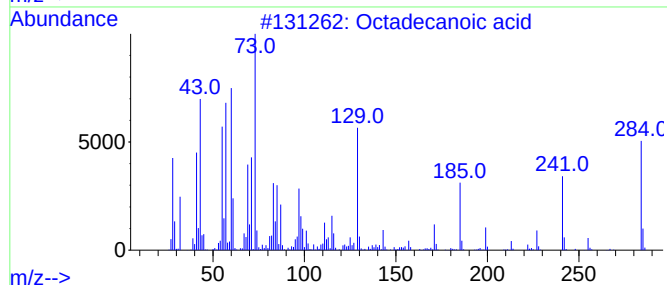
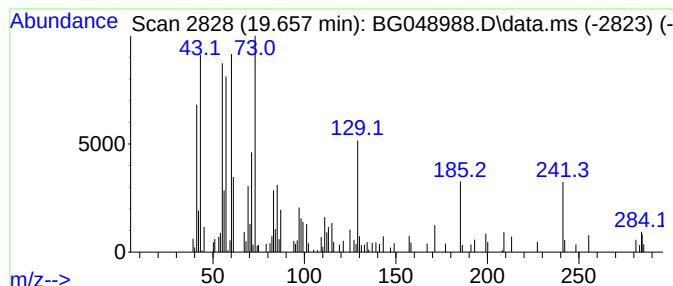
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.657	2.52 ng	83900	Chrysene-d12	21.796

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	70



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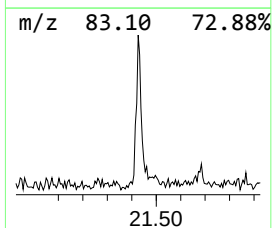
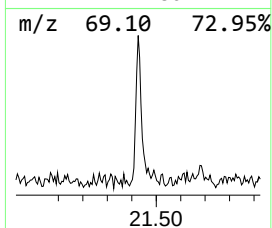
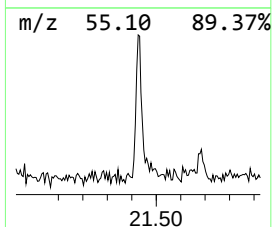
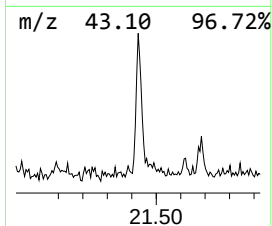
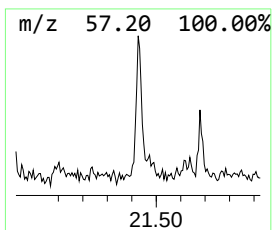
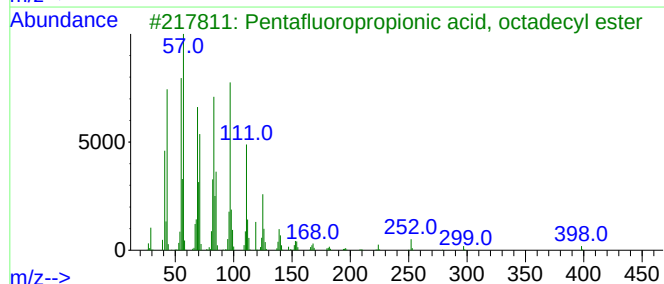
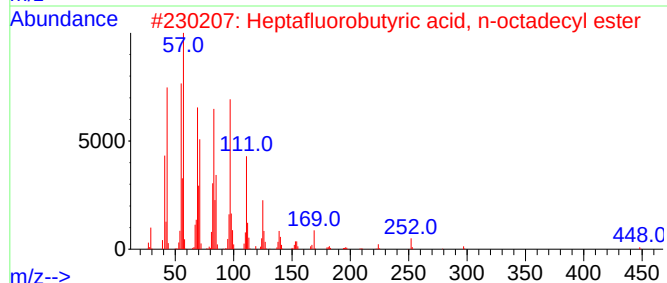
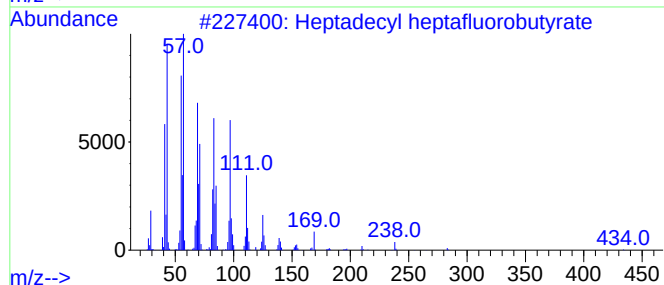
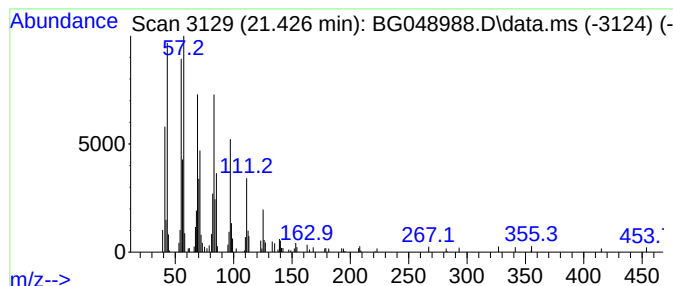
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.426	4.88 ng	162296	Chrysene-d12	21.796

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2			Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	91
3			Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	91
4			Pentafluoropropionic acid, heptafluorobutyrate	402	C20H35F5O2	959218-78-1	91
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048988.D
Acq On : 15 Jun 2021 22:06
Operator : CG/JU
Sample : M2672-12
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(52-56)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-chlor...	3.159	21.1	ng	221422	1	8.112	209468	20.0
3-Penten-2-ol	3.283	6.7	ng	69954	1	8.112	209468	20.0
2-Pentanone, 4-...	5.198	2.3	ng	23853	1	8.112	209468	20.0
Pentadecanoic acid	18.388	4.6	ng	129775	4	17.501	562648	20.0
Octadecanoic acid	19.657	2.5	ng	83900	5	21.796	665020	20.0
Heptadecyl hept...	21.426	4.9	ng	162296	5	21.796	665020	20.0