

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091422\
 Data File : BG054941.D
 Acq On : 14 Sep 2022 13:16
 Operator : CG/JU
 Sample : N4579-15
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CHERRY-HILL-COMP-14

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-BG082522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054941.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.187	319	323	331	rVB	29314	46663	2.13%	0.410%
2	5.674	399	406	417	rBV	488821	788272	35.91%	6.920%
3	7.290	673	681	699	rBV	493983	868789	39.58%	7.627%
4	8.130	816	824	833	rVB	104075	178554	8.13%	1.568%
5	9.311	1017	1025	1034	rBV	275565	516383	23.52%	4.533%
6	10.710	1254	1263	1279	rBV	74595	159391	7.26%	1.399%
7	10.962	1298	1306	1313	rBV	151910	272878	12.43%	2.396%
8	13.395	1712	1720	1728	rBV	924770	1418337	64.61%	12.452%
9	14.676	1932	1938	1943	rBV	27055	42576	1.94%	0.374%
10	14.770	1945	1954	1961	rBV	289434	476724	21.72%	4.185%
11	16.262	2201	2208	2224	rBV	767509	1237952	56.39%	10.868%
12	16.421	2227	2235	2236	rBV2	36185	61077	2.78%	0.536%
13	16.462	2236	2242	2248	rVB	191363	321003	14.62%	2.818%
14	16.896	2310	2316	2332	rBV3	34296	84047	3.83%	0.738%
15	17.519	2416	2422	2428	rBV	403006	601158	27.39%	5.278%
16	18.154	2526	2530	2535	rBV	29496	38013	1.73%	0.334%
17	18.683	2615	2620	2629	rBV3	29409	69154	3.15%	0.607%
18	18.806	2636	2641	2654	rVB2	37865	103030	4.69%	0.905%
19	20.057	2848	2854	2859	rBV2	48646	109188	4.97%	0.959%
20	20.116	2859	2864	2871	rVB	1615922	2195149	100.00%	19.271%
21	20.992	3007	3013	3020	rVB2	45207	96792	4.41%	0.850%
22	21.415	3081	3085	3097	rBV4	31371	81887	3.73%	0.719%
23	21.814	3146	3153	3164	rVB2	389883	675798	30.79%	5.933%
24	21.955	3170	3177	3178	rBV3	33306	68444	3.12%	0.601%
25	22.602	3283	3287	3292	rBV	27123	41696	1.90%	0.366%
26	23.318	3406	3409	3416	rVB2	19784	37103	1.69%	0.326%
27	24.164	3549	3553	3563	rVB3	20607	43820	2.00%	0.385%
28	24.311	3571	3578	3579	rBV2	18559	33631	1.53%	0.295%
29	25.187	3717	3727	3740	rVB2	230223	723157	32.94%	6.349%

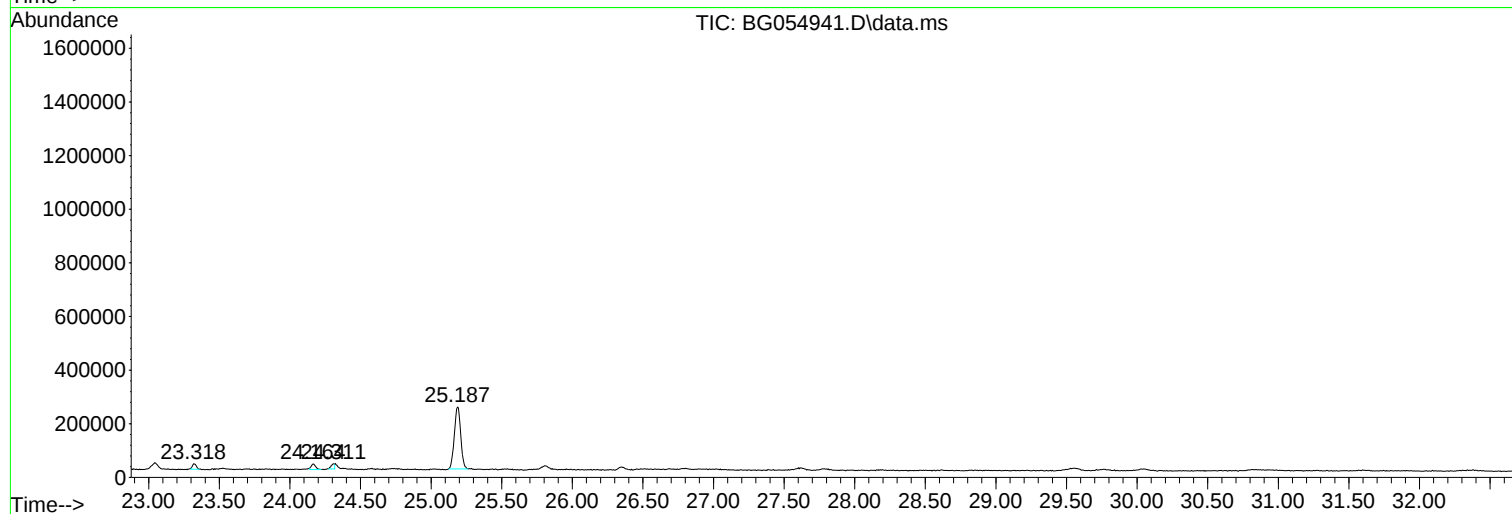
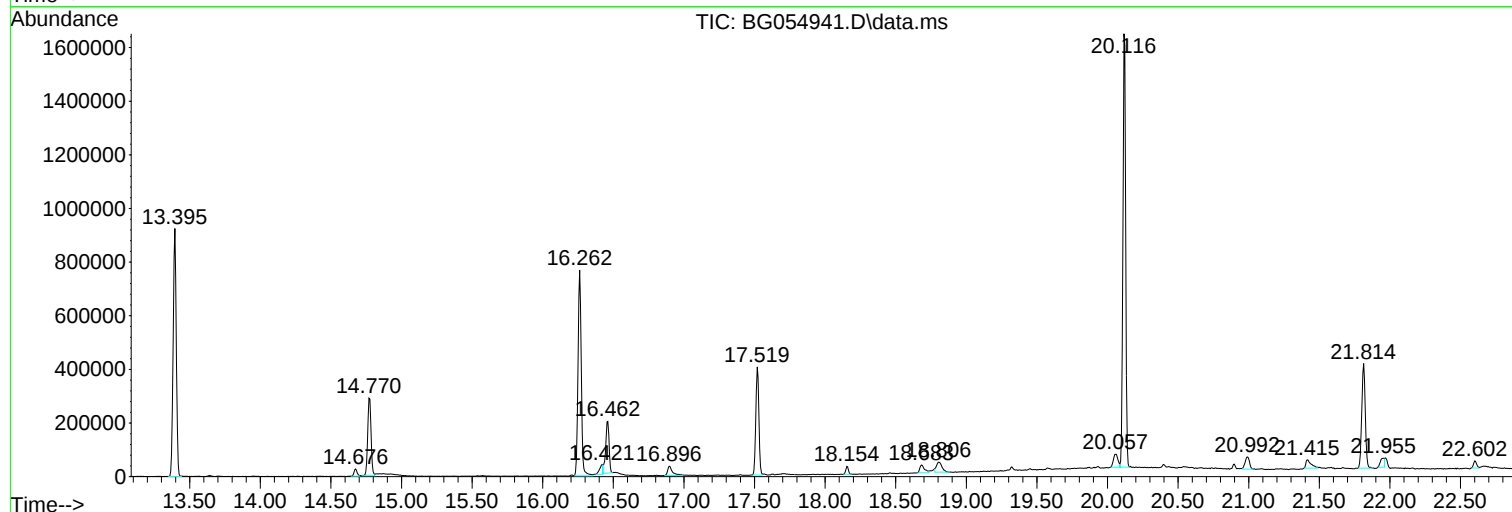
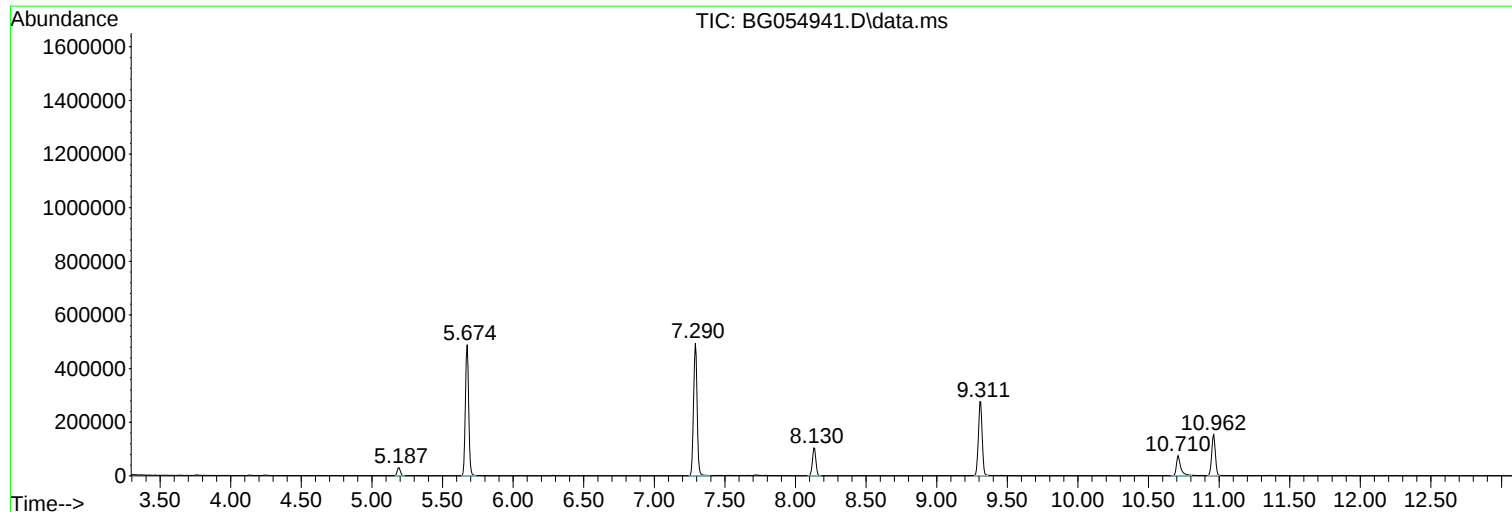
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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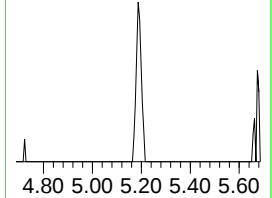
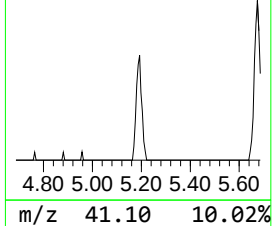
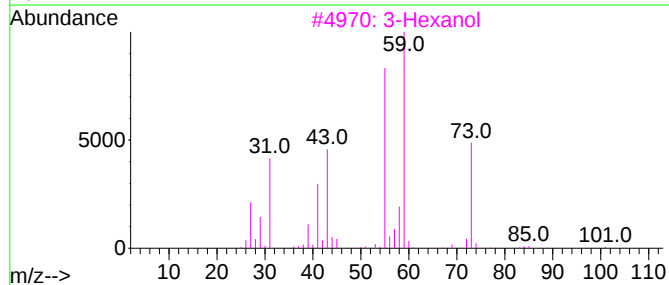
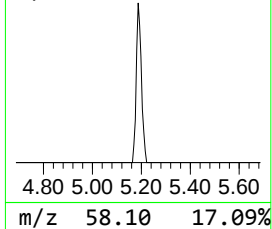
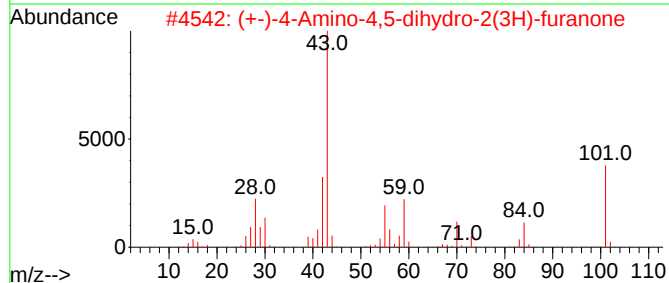
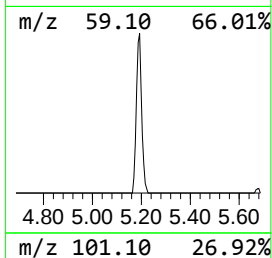
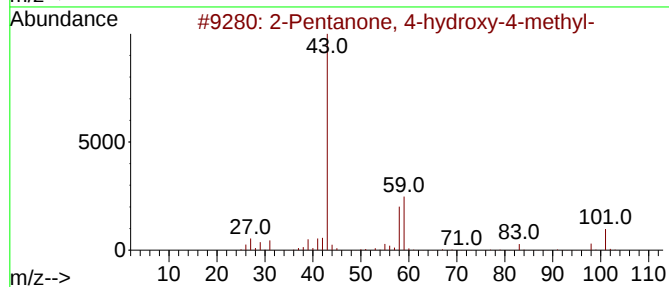
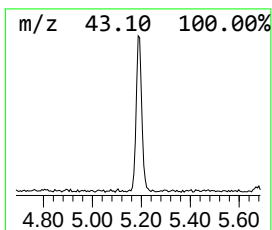
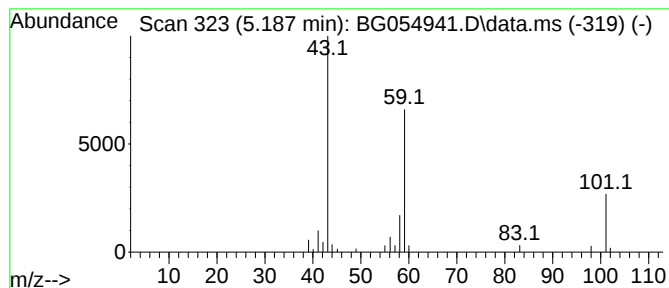
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.187	5.23 ng	46663	1,4-Dichlorobenzene-d4		8.130	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	72
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...		101	C4H7NO2	016504-58-8	47
3	3-Hexanol		102	C6H14O	000623-37-0	28
4	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	25
5	1,2-Butanediol		90	C4H10O2	000584-03-2	23



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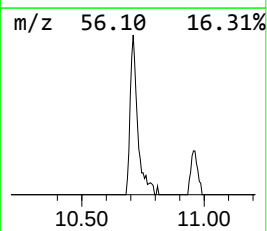
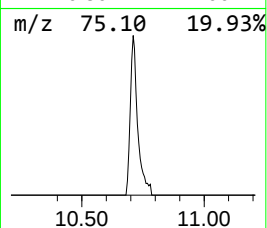
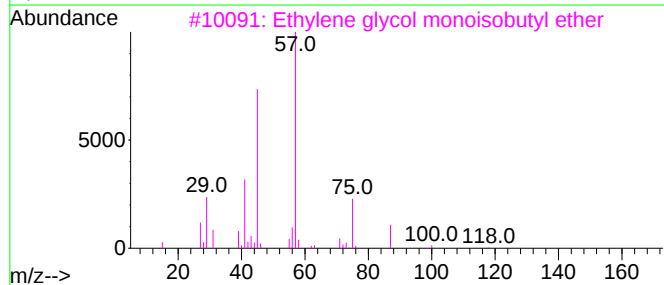
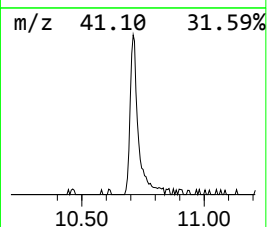
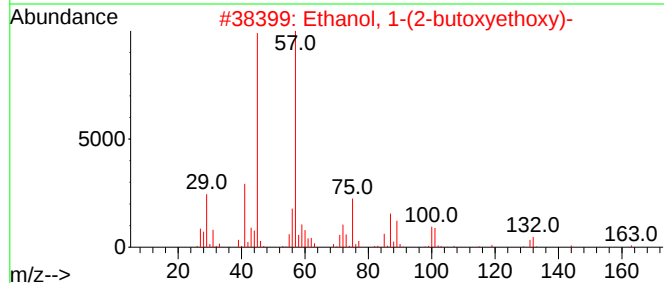
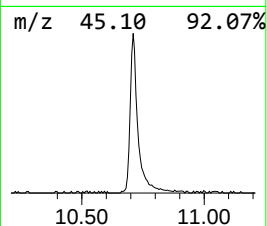
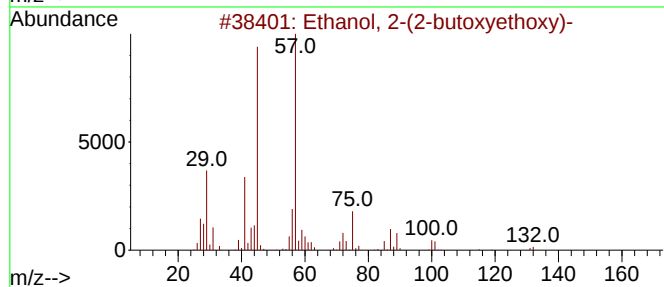
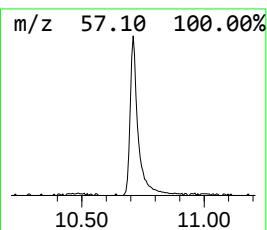
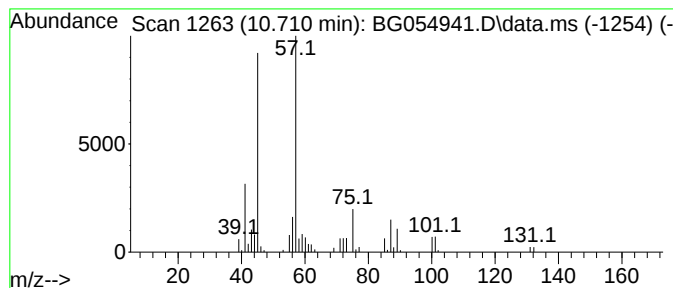
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.710	11.68 ng	159391	Naphthalene-d8	10.962

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	53
5			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53



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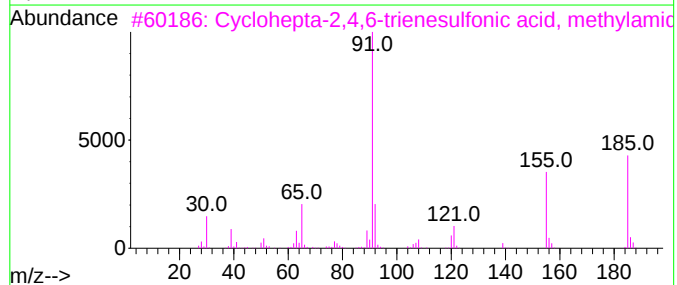
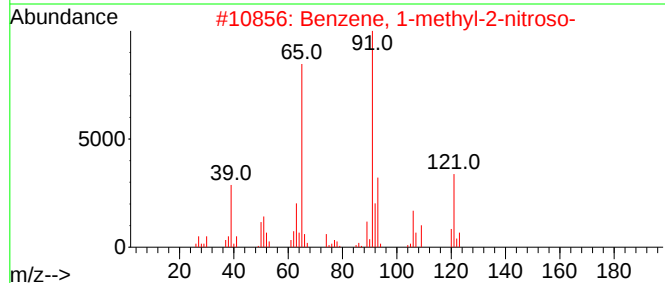
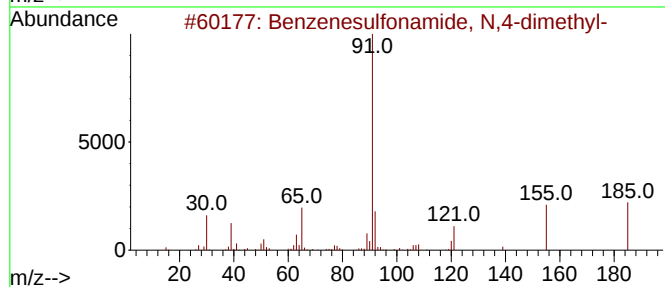
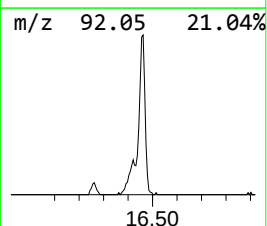
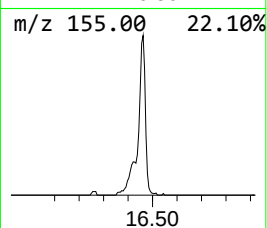
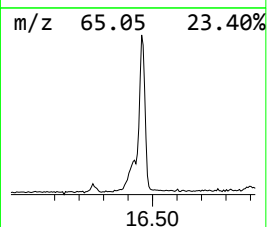
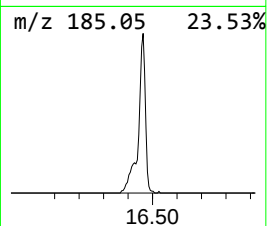
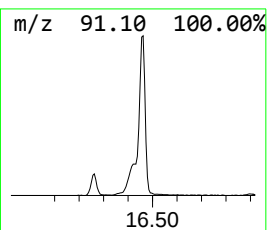
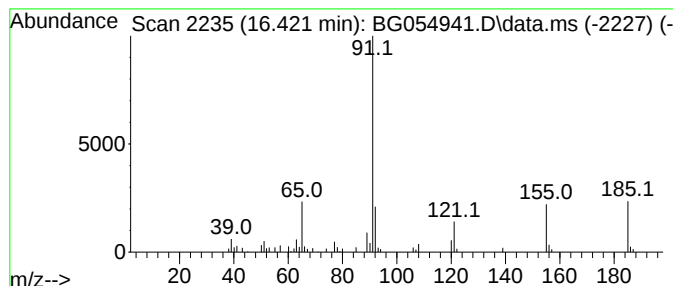
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzenesulfonamide, N,4-dim... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.421	2.03 ng	61077	Phenanthrene-d10	17.519

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	95
2			Benzene, 1-methyl-2-nitroso-	121	C7H7NO	000611-23-4	64
3			Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	58
4			4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	47
5			(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	47



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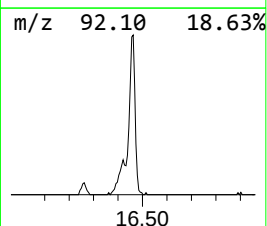
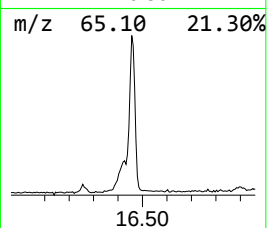
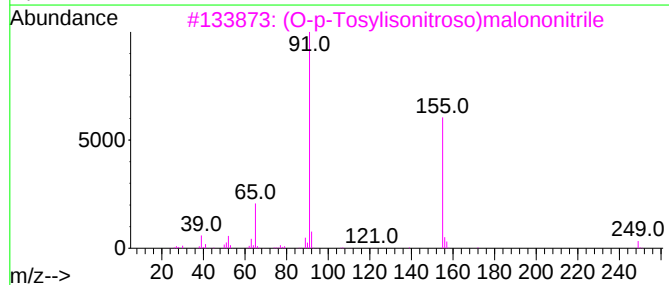
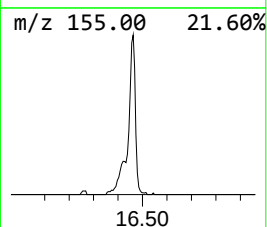
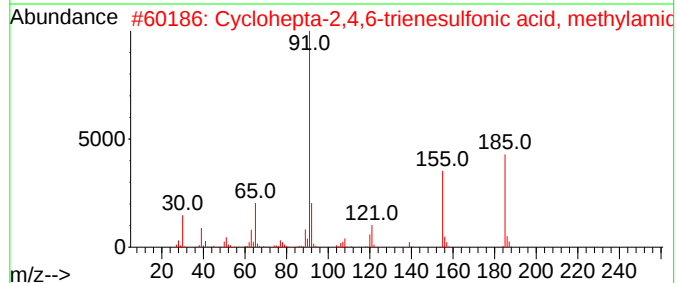
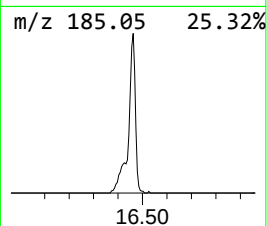
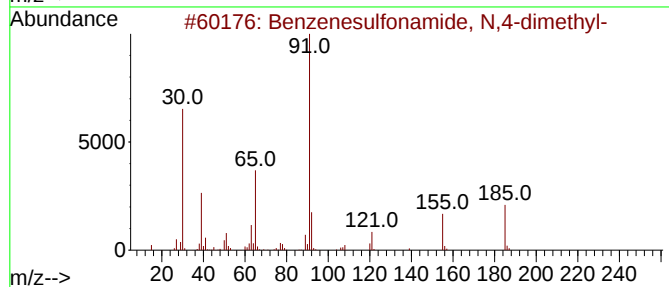
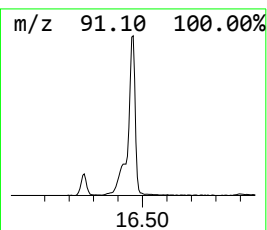
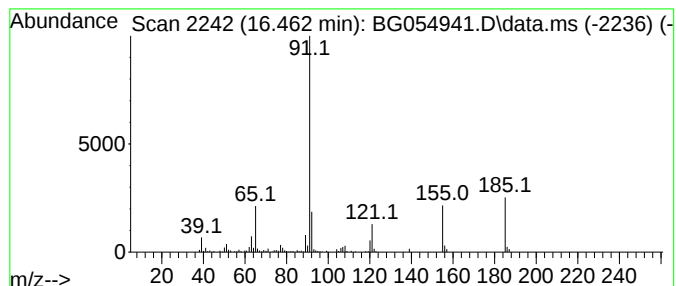
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Peak Number 4 Cyclohepta-2,4,6-trienesulf... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.462	10.68 ng	321003	Phenanthrene-d10	17.519

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	95
2			Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	68
3			(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	47
4			4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	47
5			p-Toluenesulfonylacetonitrile	195	C9H9NO2S	005697-44-9	47



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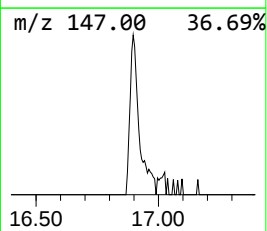
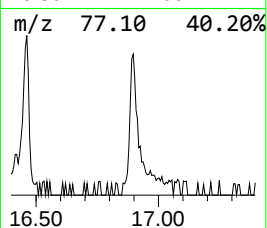
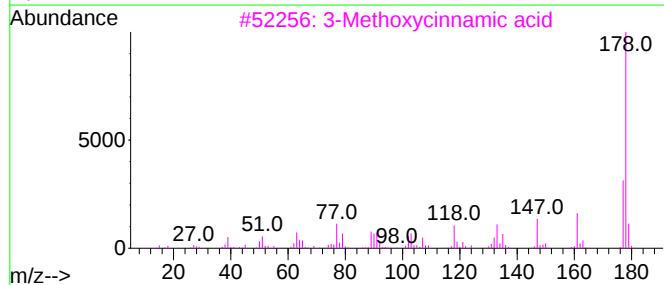
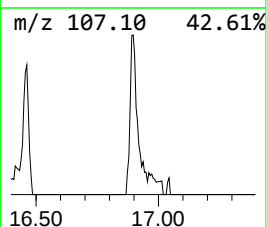
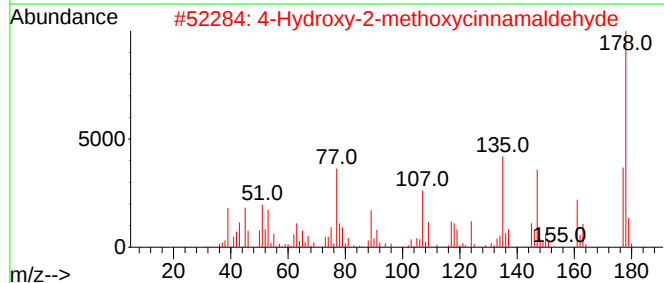
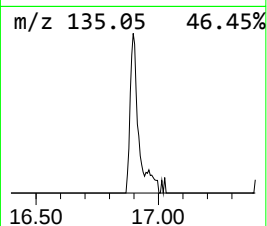
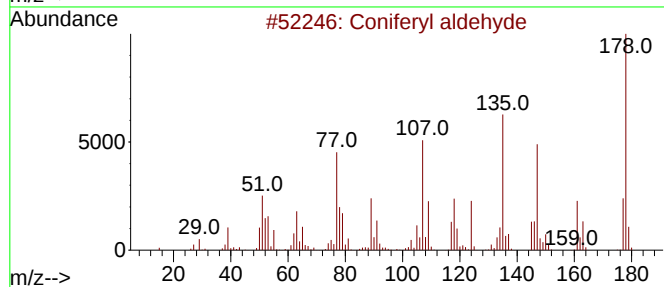
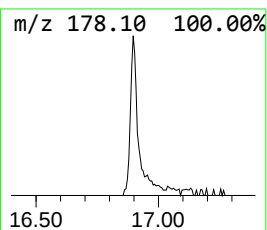
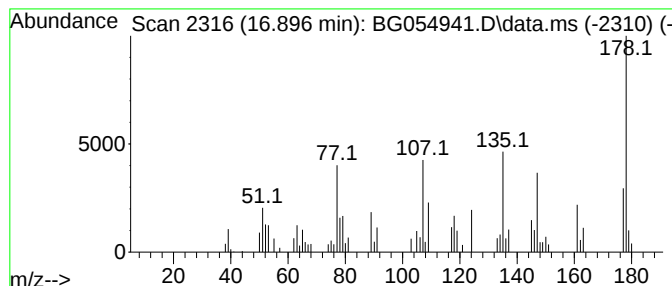
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Peak Number 5 Coniferyl aldehyde Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.897	2.80 ng	84047	Phenanthrene-d10	17.519

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Coniferyl aldehyde	178	C10H10O3	000458-36-6	98
2			4-Hydroxy-2-methoxycinnamaldehyde	178	C10H10O3	127321-19-1	97
3			3-Methoxycinnamic acid	178	C10H10O3	006099-04-3	50
4			Benzaldehyde, 4-(dimethylamino)-...	178	C10H14N2O	019293-74-4	43
5			1H-Pyrrolo[3,4-c]pyridine-1,3,4(...	178	C8H6N2O3	026413-69-4	38



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ClientSampleId :
CHERRY-HILL-COMP-14

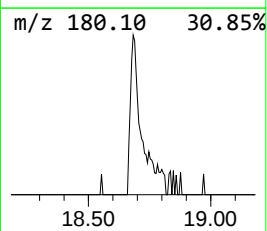
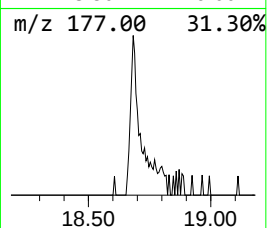
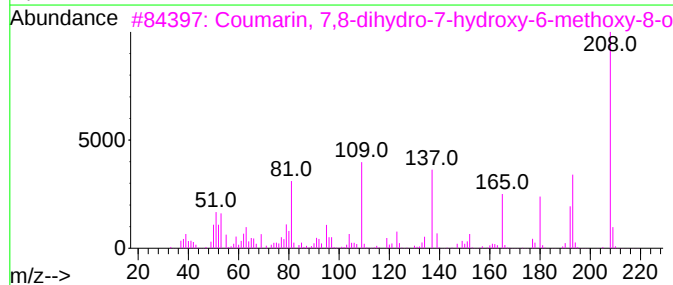
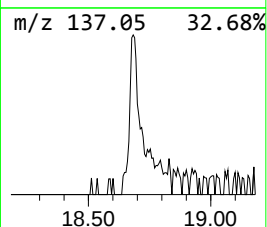
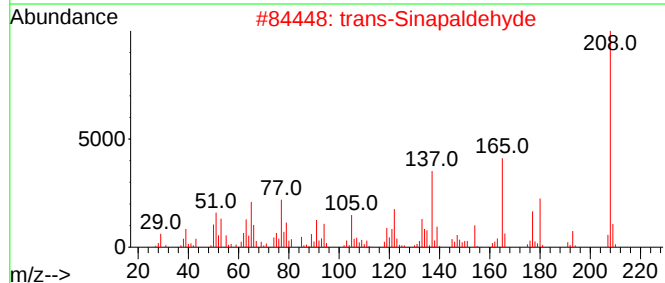
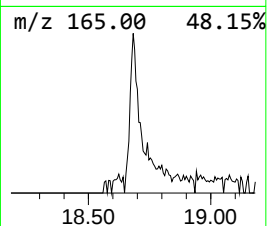
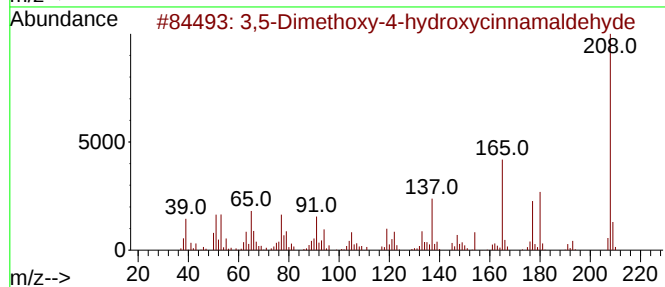
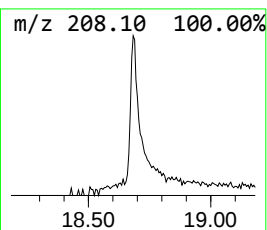
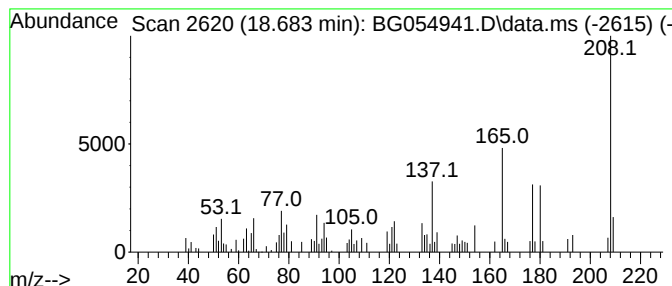
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.683	2.30 ng	69154	Phenanthrene-d10	17.519

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3,5-Dimethoxy-4-hydroxycinnamal... 208	C11H12O4		087345-53-7	98
2		trans-Sinapaldehyde 208	C11H12O4		004206-58-0	93
3		Coumarin, 7,8-dihydro-7-hydroxy-... 208	C10H8O5		1000263-13-6	58
4		2-Allyl-3-ethoxy-4-methoxyphenol 208	C12H16O3		1000122-70-6	58
5		2H-1-Benzopyran-2-one, 7,8-dihyd... 208	C10H8O5		000574-84-5	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091422\
Data File : BG054941.D
Acq On : 14 Sep 2022 13:16
Operator : CG/JU
Sample : N4579-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHERRY-HILL-COMP-14

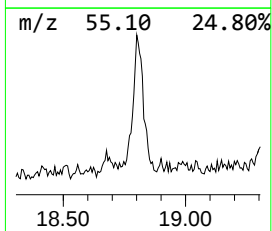
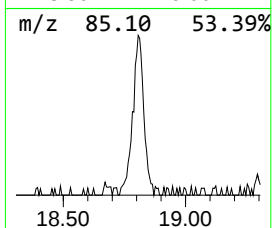
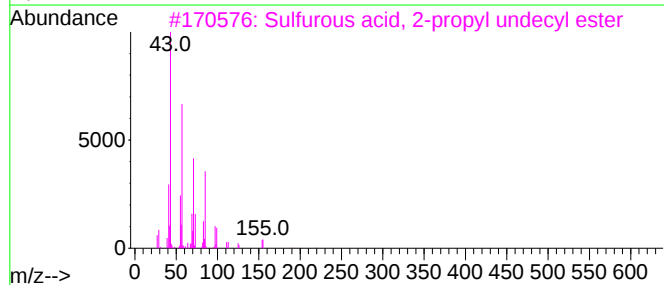
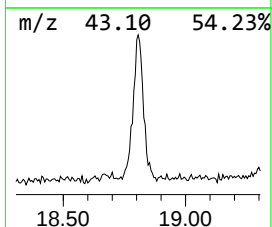
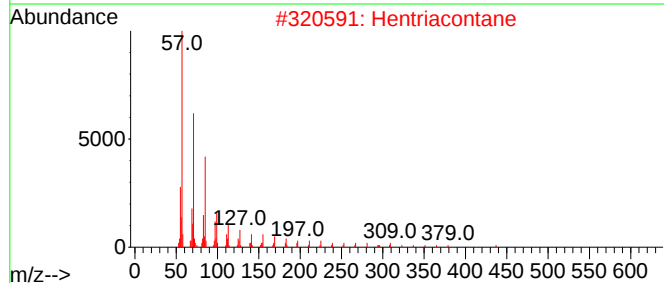
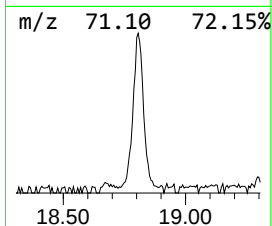
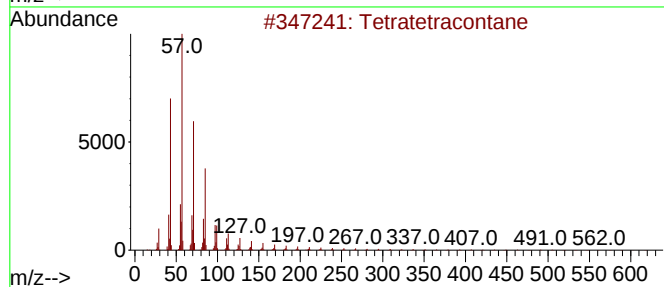
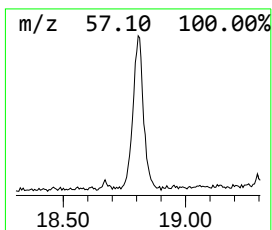
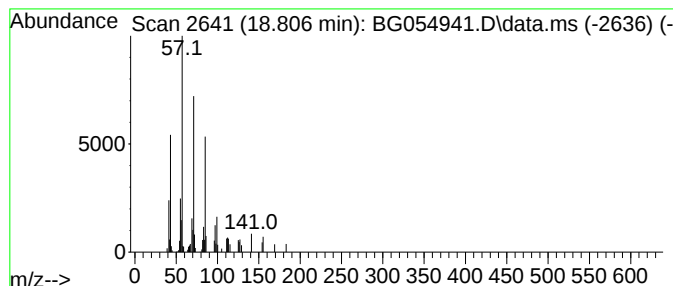
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetratetracontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.806	3.43 ng	103030	Phenanthrene-d10	17.519

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Hentriacontane	437	C31H64	000630-04-6	86
3			Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	86
4			Hexacosane	366	C26H54	000630-01-3	86
5			Octacosane	394	C28H58	000630-02-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091422\
Data File : BG054941.D
Acq On : 14 Sep 2022 13:16
Operator : CG/JU
Sample : N4579-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CHERRY-HILL-COMP-14

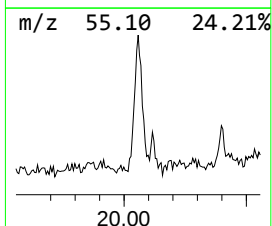
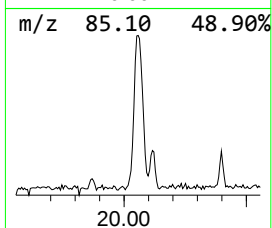
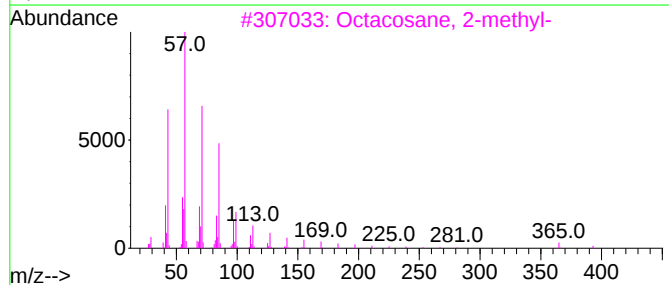
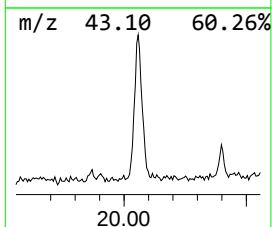
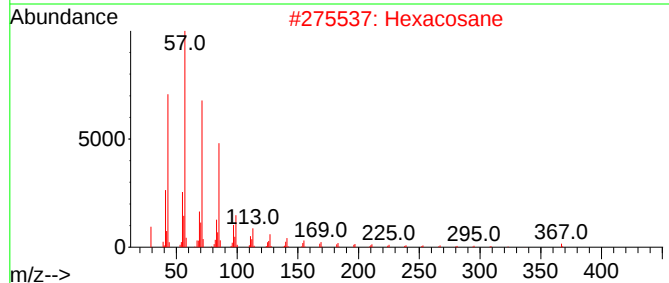
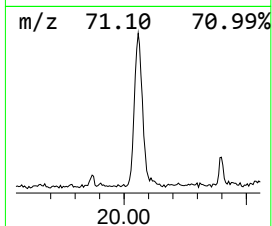
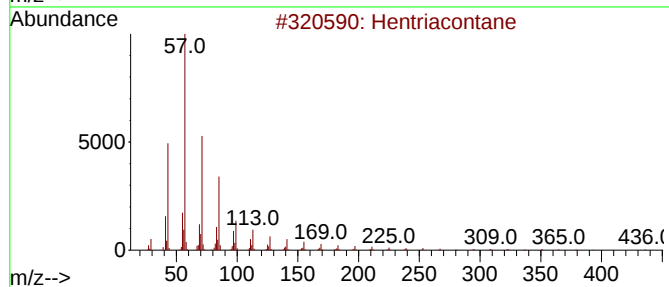
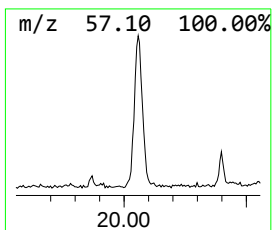
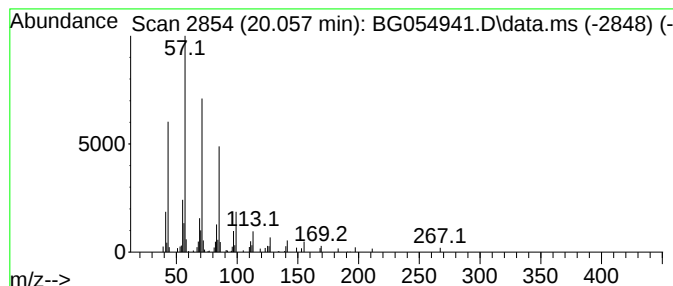
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.057	3.23 ng	109188	Chrysene-d12	21.814

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hentriacontane	437	C31H64	000630-04-6	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4		Triacontane	422	C30H62	000638-68-6	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091422\
Data File : BG054941.D
Acq On : 14 Sep 2022 13:16
Operator : CG/JU
Sample : N4579-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CHERRY-HILL-COMP-14

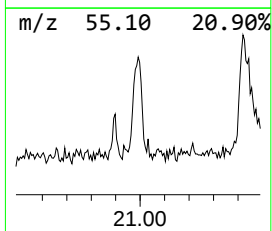
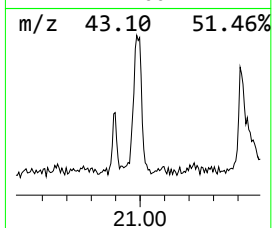
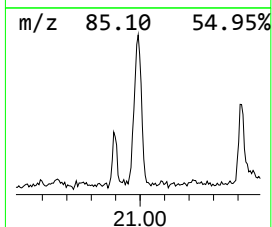
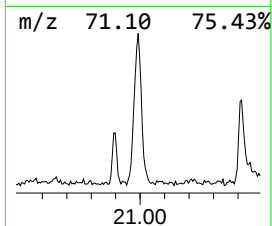
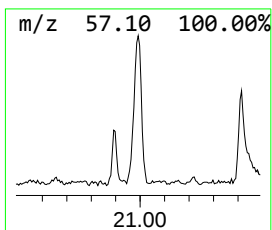
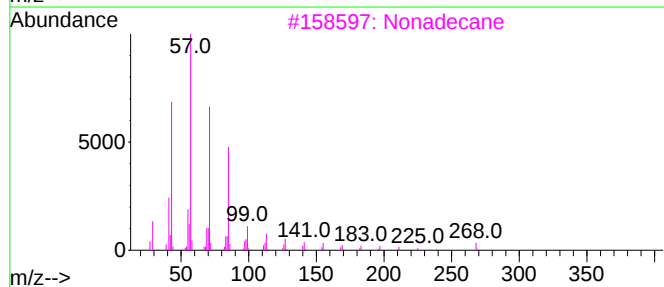
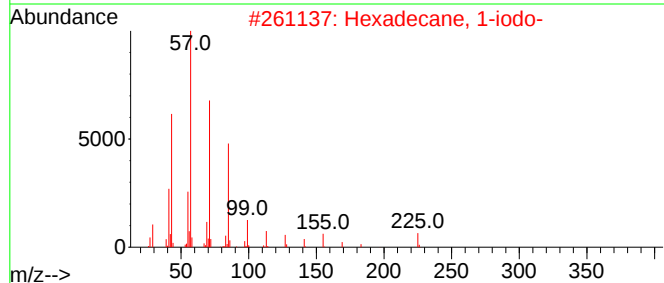
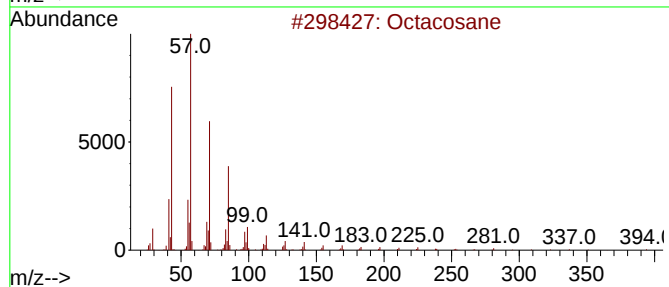
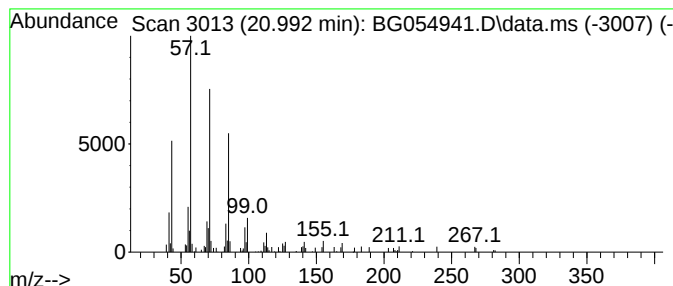
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.992	2.86 ng	96792	Chrysene-d12	21.814

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90
3			Nonadecane	268	C19H40	000629-92-5	87
4			Pentacosane	352	C25H52	000629-99-2	87
5			Docosane	310	C22H46	000629-97-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091422\
Data File : BG054941.D
Acq On : 14 Sep 2022 13:16
Operator : CG/JU
Sample : N4579-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CHERRY-HILL-COMP-14

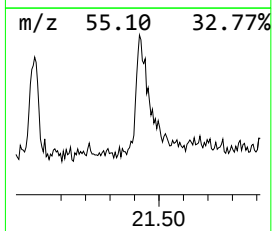
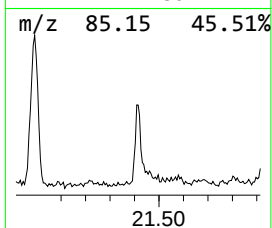
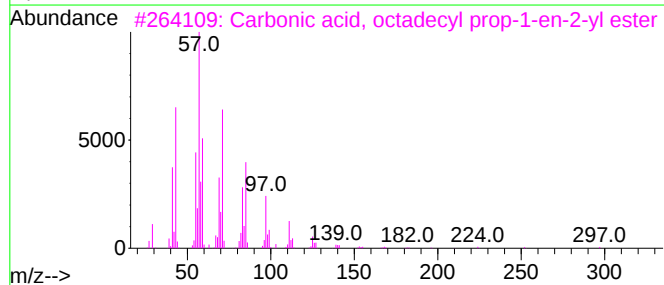
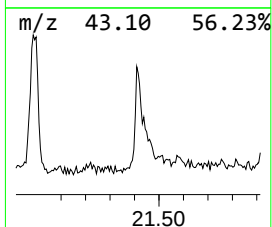
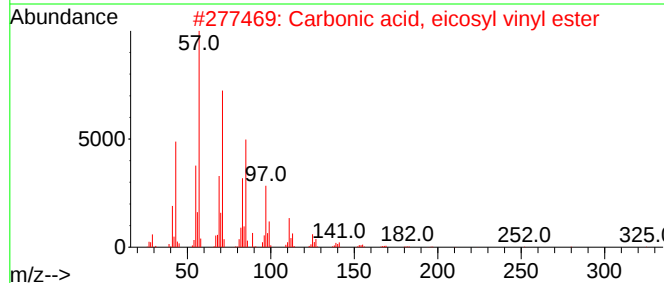
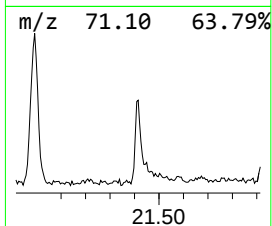
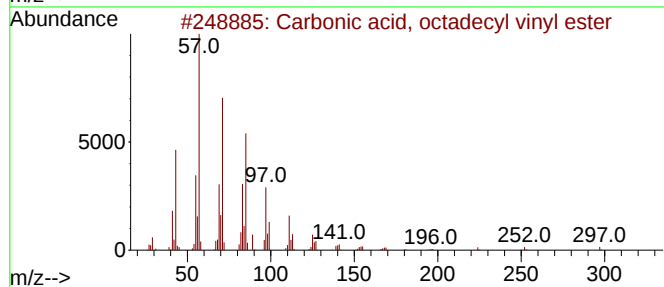
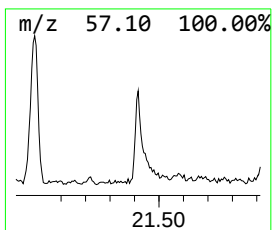
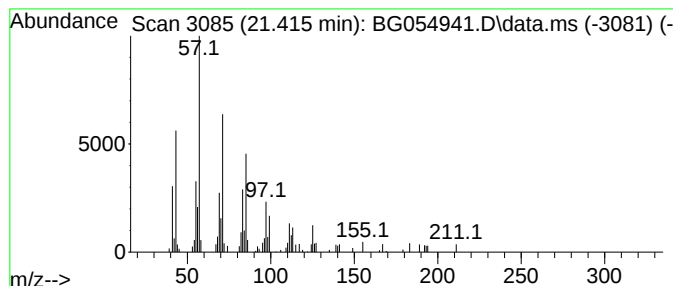
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Carbonic acid, octadecyl vi... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.415	2.42 ng	81887	Chrysene-d12	21.814

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	91
2			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91
3			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
4			Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1010309-12-5	90
5			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091422\
Data File : BG054941.D
Acq On : 14 Sep 2022 13:16
Operator : CG/JU
Sample : N4579-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CHERRY-HILL-COMP-14

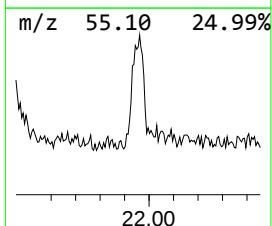
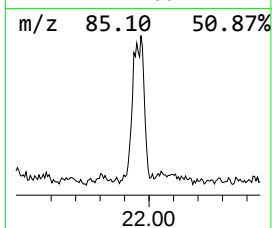
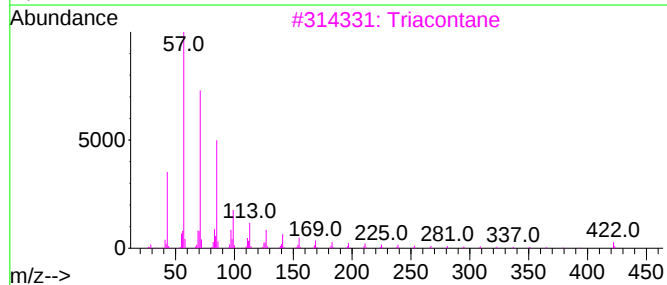
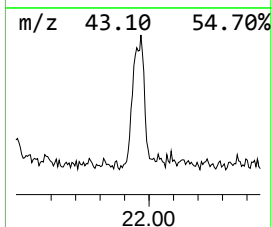
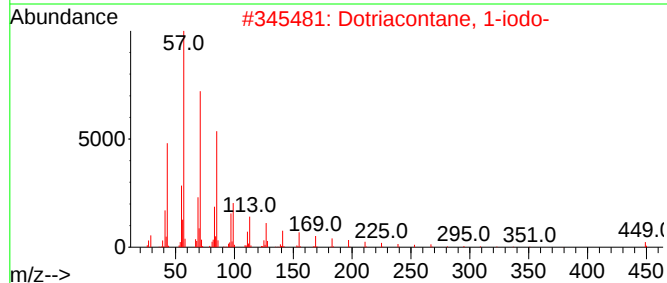
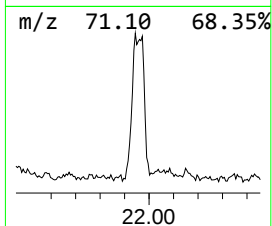
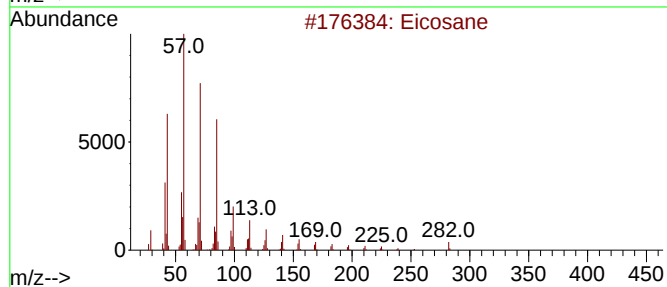
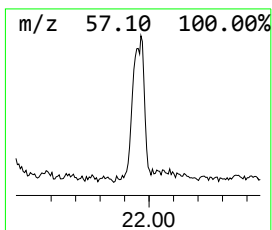
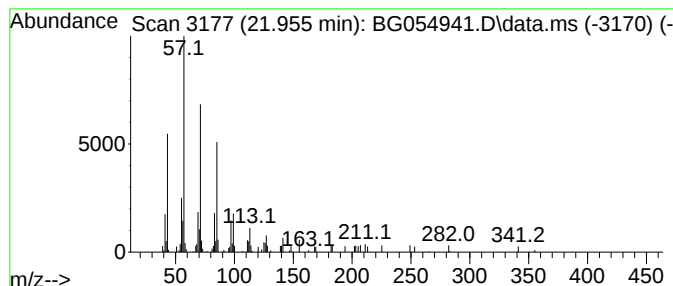
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.955	2.03 ng	68444	Chrysene-d12	21.814

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	96
2			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
3			Triacontane	422	C30H62	000638-68-6	91
4			Docosane, 11-decyl-	451	C32H66	055401-55-3	91
5			Tetratetracontane	619	C44H90	007098-22-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091422\
Data File : BG054941.D
Acq On : 14 Sep 2022 13:16
Operator : CG/JU
Sample : N4579-15
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CHERRY-HILL-COMP-14

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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
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Ethanol, 2-(2-b...	10.710	11.7	ng	159391	2	10.962	272878	20.0
Benzenesulfonam...	16.421	2.0	ng	61077	4	17.519	601158	20.0
Cyclohepta-2,4,...	16.462	10.7	ng	321003	4	17.519	601158	20.0
Coniferyl aldehyde	16.897	2.8	ng	84047	4	17.519	601158	20.0
3,5-Dimethoxy-4...	18.683	2.3	ng	69154	4	17.519	601158	20.0
Tetratetracontane	18.806	3.4	ng	103030	4	17.519	601158	20.0
Hentriacontane	20.057	3.2	ng	109188	5	21.814	675798	20.0
Octacosane	20.992	2.9	ng	96792	5	21.814	675798	20.0
Carbonic acid, ...	21.415	2.4	ng	81887	5	21.814	675798	20.0
Eicosane	21.955	2.0	ng	68444	5	21.814	675798	20.0