

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM072122\
 Data File : BM035900.D
 Acq On : 21 Jul 2022 22:00
 Operator : CG/JU
 Sample : N3810-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 COMP-2

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_M\Methods\8270-BM071822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035900.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.451	396	402	410	rBV	2825572	3959229	17.16%	3.536%
2	5.540	411	417	437	rVB2	67420	264934	1.15%	0.237%
3	7.057	667	675	687	rBV	2765275	4135994	17.93%	3.694%
4	7.893	810	817	825	rBV	1266607	1926785	8.35%	1.721%
5	9.057	1008	1015	1024	rBV	1592882	2570102	11.14%	2.296%
6	10.698	1285	1294	1300	rBV	1620120	2629743	11.40%	2.349%
7	13.157	1705	1712	1721	rVB	3734279	5340117	23.15%	4.770%
8	14.527	1938	1945	1951	rBV	2098444	2967576	12.86%	2.651%
9	15.098	2034	2042	2066	rBV2	101900	569428	2.47%	0.509%
10	16.010	2190	2197	2205	rBV	2372981	3274196	14.19%	2.924%
11	17.268	2404	2411	2415	rBV	2278534	3281252	14.22%	2.931%
12	17.310	2415	2418	2423	rVB	475608	612285	2.65%	0.547%
13	19.321	2755	2760	2765	rBV	998505	1253796	5.43%	1.120%
14	19.680	2817	2821	2830	rVB	872676	1213788	5.26%	1.084%
15	19.886	2851	2856	2868	rVB	5515434	6719891	29.13%	6.002%
16	20.098	2889	2892	2896	rBV	208964	249184	1.08%	0.223%
17	21.162	3070	3073	3079	rBV2	377490	468628	2.03%	0.419%
18	21.439	3114	3120	3124	rBV2	3114409	4663371	20.21%	4.165%
19	21.474	3124	3126	3135	rVB	537754	732437	3.17%	0.654%
20	23.092	3396	3401	3408	rBV2	435782	1230972	5.34%	1.099%
21	23.603	3485	3488	3496	rVB	267957	464795	2.01%	0.415%
22	23.709	3501	3506	3515	rVB	399118	806951	3.50%	0.721%
23	23.815	3517	3524	3531	rBV2	1924566	3861817	16.74%	3.449%
24	24.703	3670	3675	3690	rVB	530343	1216211	5.27%	1.086%
25	27.650	4169	4176	4196	rVB2	650230	2531784	10.97%	2.261%
26	28.062	4237	4246	4262	rVB2	864772	3158047	13.69%	2.821%
27	28.262	4266	4280	4313	rVB8	3302079	19435270	84.24%	17.359%
28	28.668	4334	4349	4356	rBV3	5416311	23070709	100.00%	20.606%
29	29.050	4403	4414	4437	rVB2	1715560	9350843	40.53%	8.352%

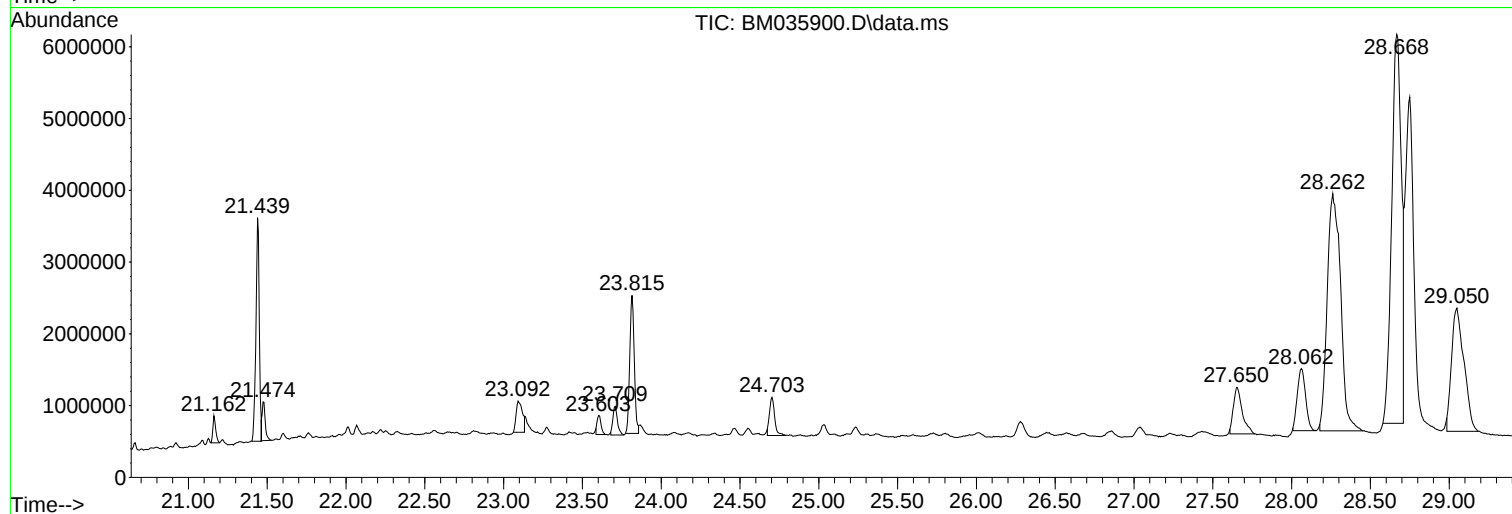
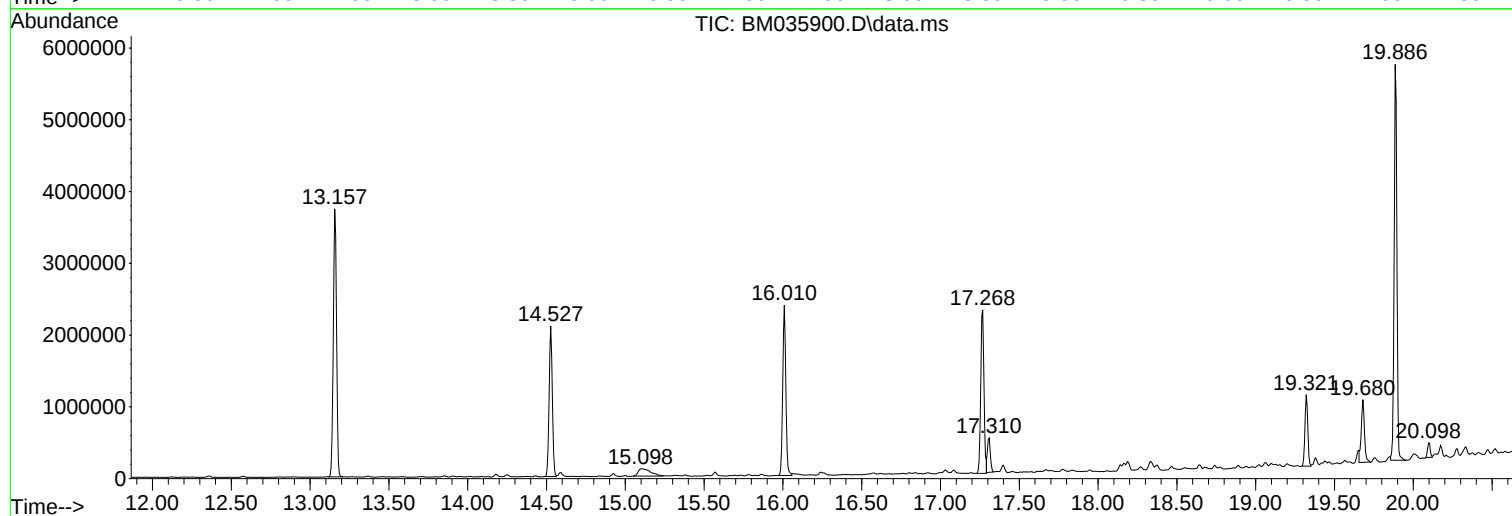
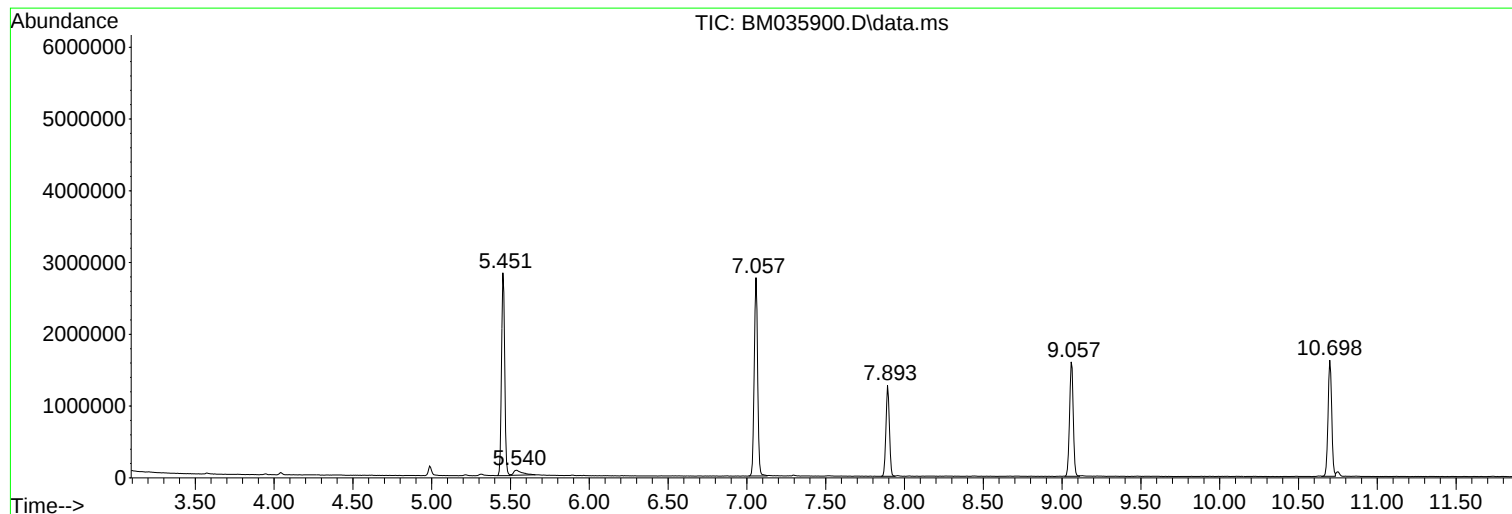
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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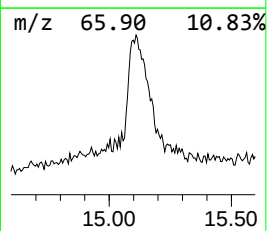
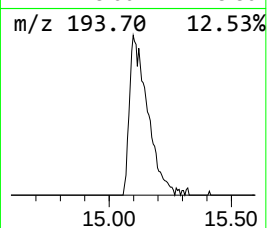
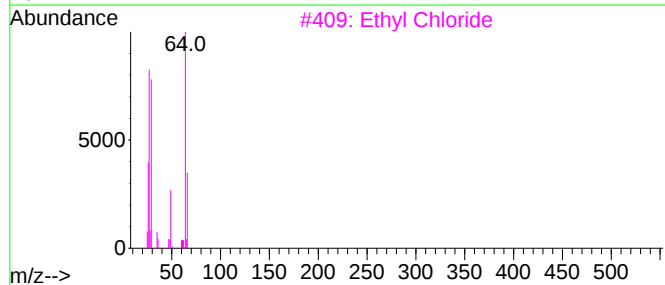
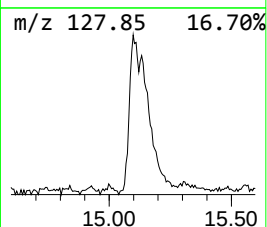
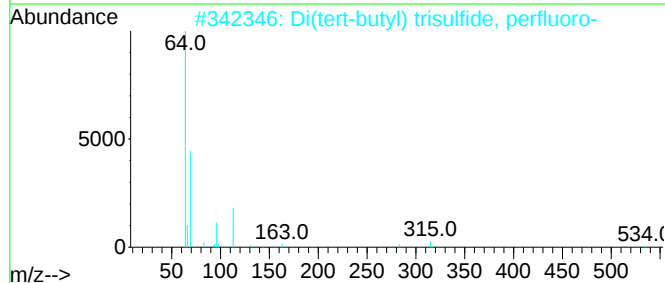
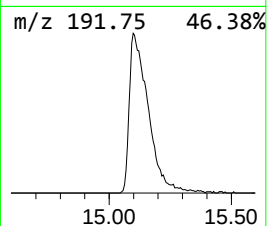
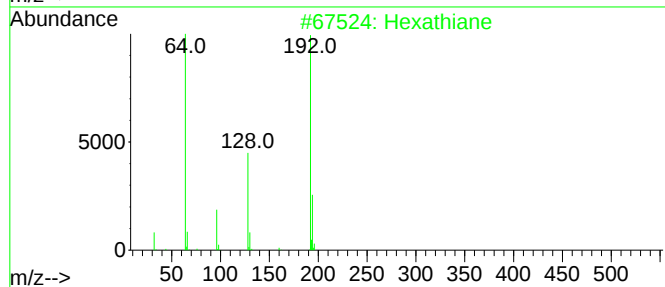
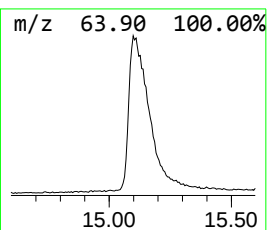
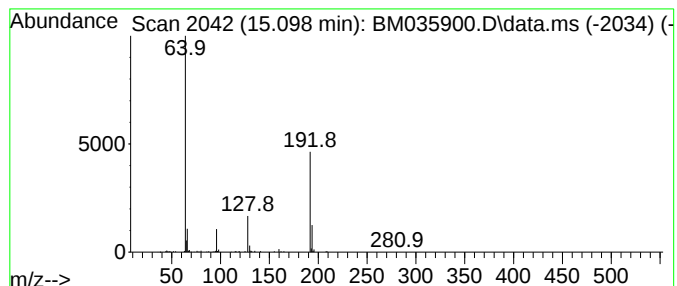
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexathiane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.098	3.84 ng	569428	Acenaphthene-d10	14.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexathiane	192	S6	013798-23-7	90
2			Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	39
3			Ethyl Chloride	64	C2H5Cl	000075-00-3	5
4			Sulfur dioxide	64	O2S	007446-09-5	4
5			Tetrazolo[1,5-b]pyridazine, 6-ch...	155	C4H2ClN5	021413-15-0	4



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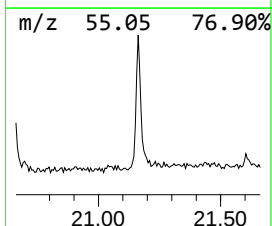
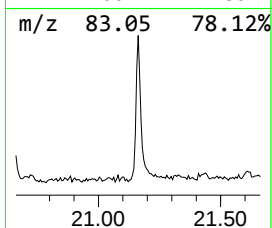
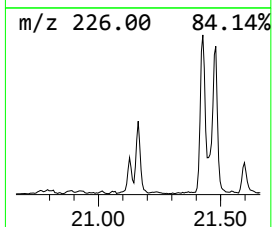
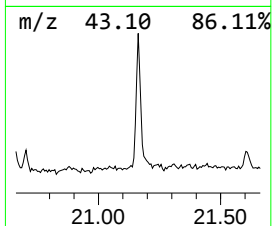
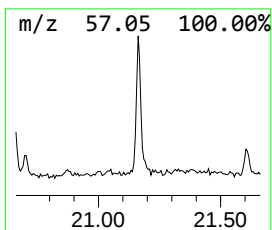
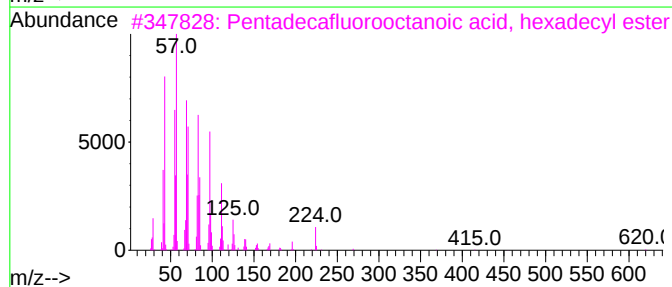
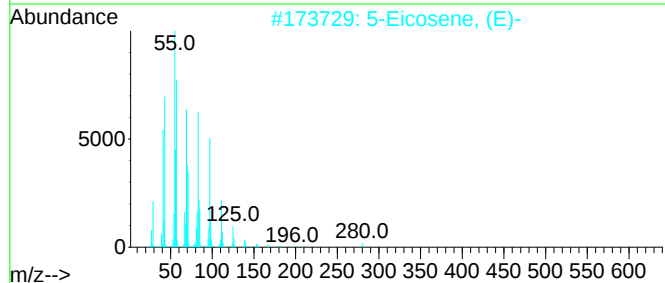
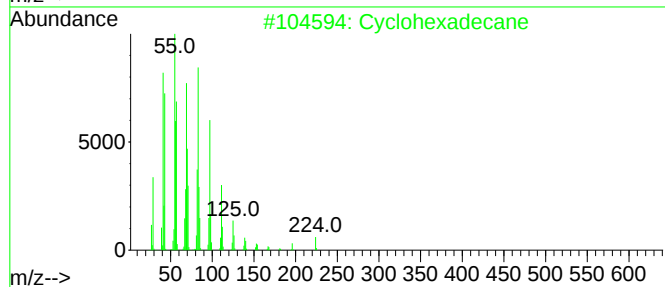
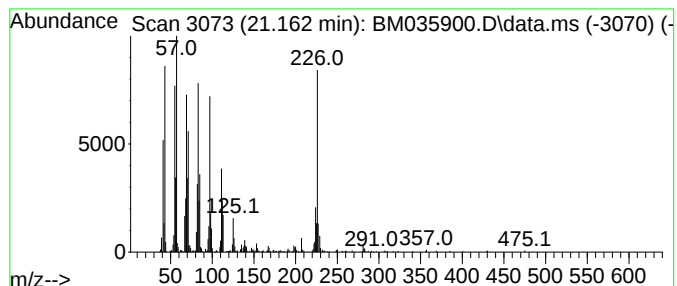
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Peak Number 3 Cyclohexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.162	2.01 ng	468628	Chrysene-d12	21.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	95
2			5-Eicosene, (E)-	280	C20H40	074685-30-6	95
3			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	86
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	83
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64



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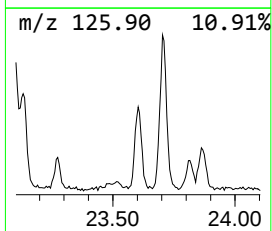
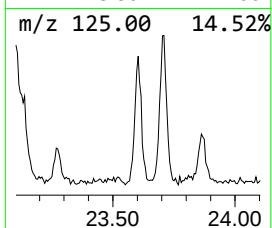
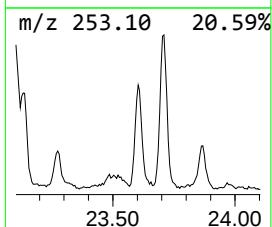
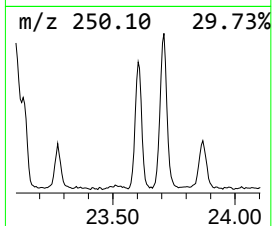
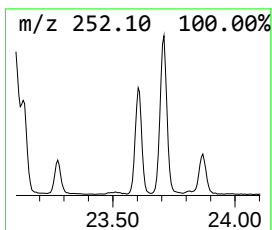
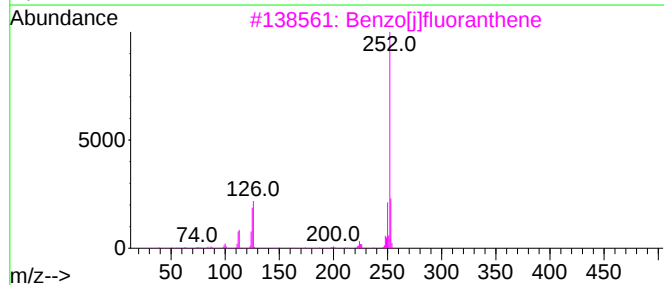
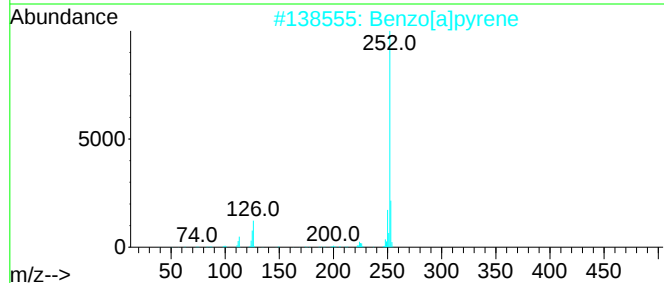
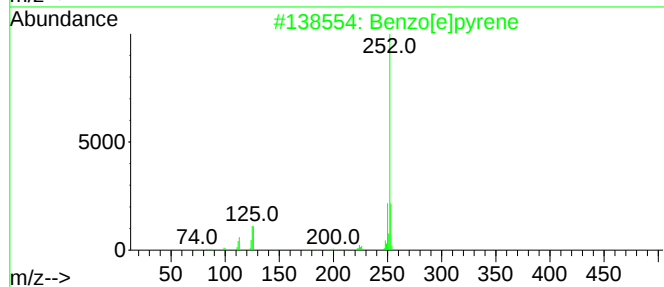
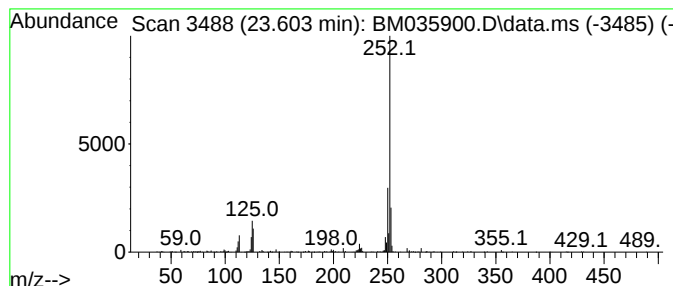
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.603	2.41 ng	464795	Perylene-d12	23.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	99
2			Benzo[a]pyrene	252	C20H12	000050-32-8	97
3			Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93



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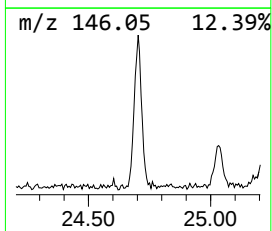
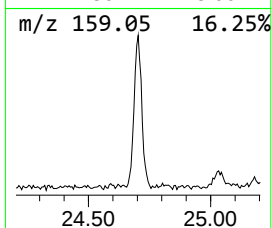
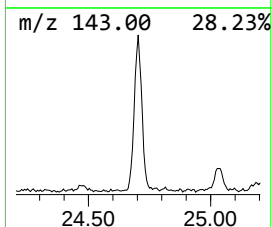
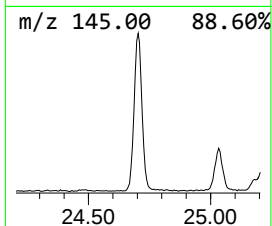
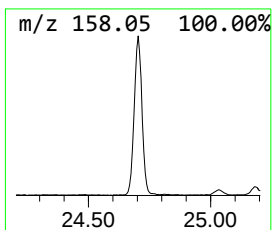
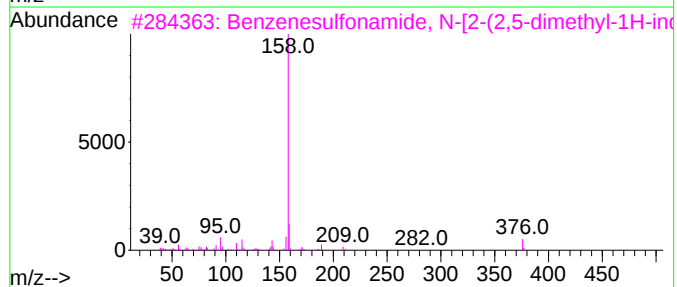
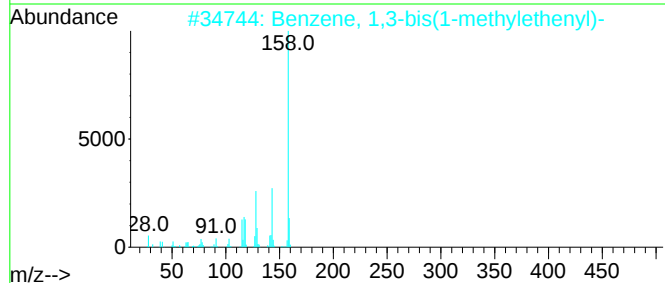
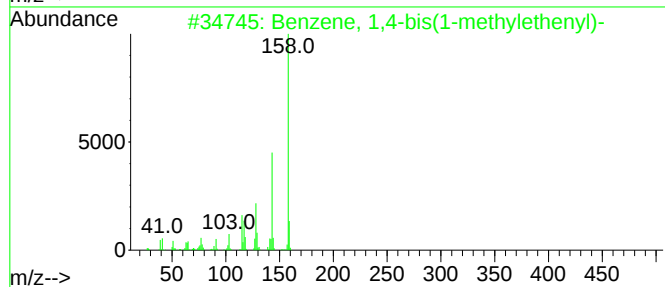
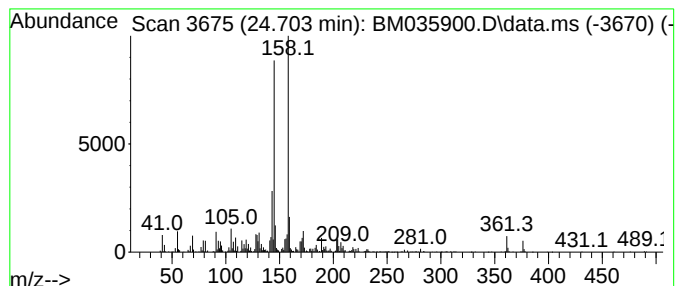
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Peak Number 5 Benzene, 1,4-bis(1-methylet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.703	6.30 ng	1216210	Perylene-d12	23.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-bis(1-methylethenyl)-	158	C12H14	001605-18-1	50
2			Benzene, 1,3-bis(1-methylethenyl)-	158	C12H14	003748-13-8	43
3			Benzenesulfonamide, N-[2-(2,5-di...	376	C19H21FN2O3S	1000304-39-3	38
4			1H-Indole-3-methanamine, 5-ethyl...	202	C13H18N2	074367-51-4	35
5			4-Chloro-2-methylthiophenol	158	C7H7ClS	017178-01-7	30



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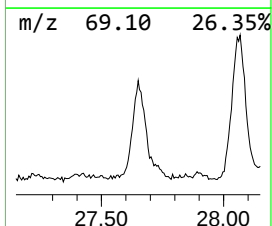
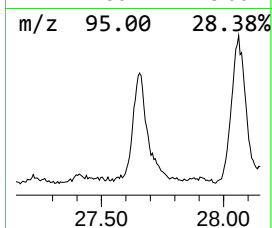
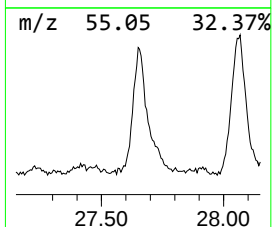
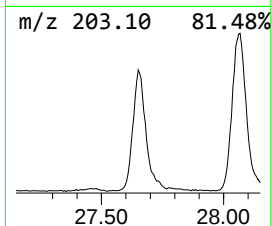
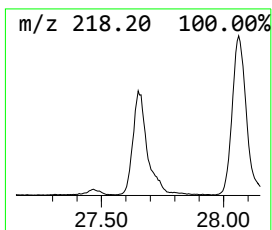
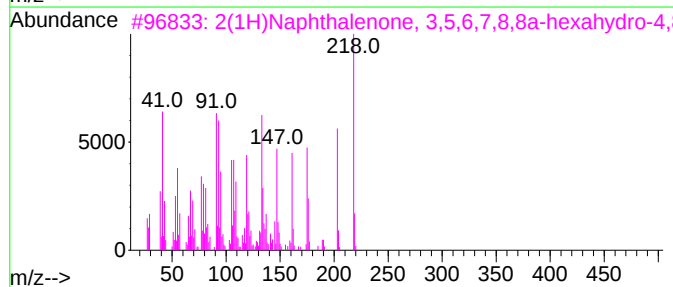
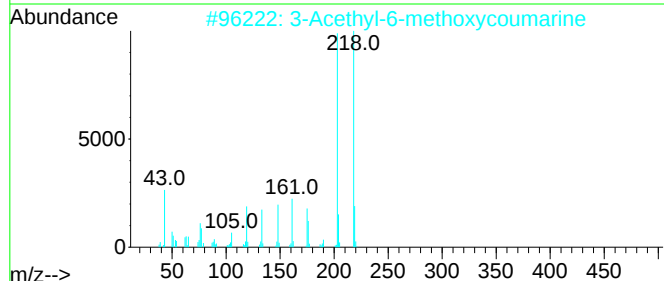
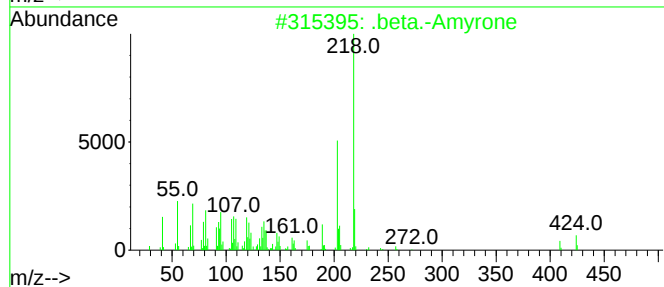
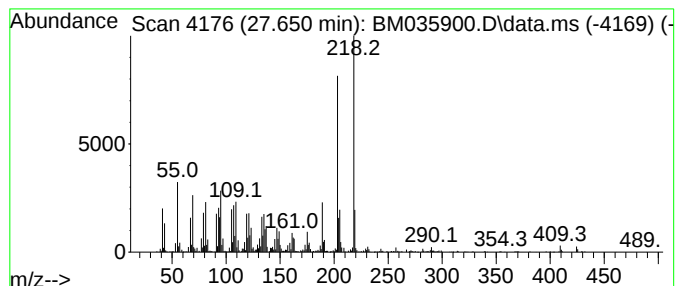
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Peak Number 6 .beta.-Amyrone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.650	13.11 ng	2531780	Perylene-d12	23.815

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Amyrone	424	C30H48O	000638-97-1	76
2		3-Acetyl-6-methoxycoumarine	218	C12H10O4	013252-80-7	58
3		2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	58
4		Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	55
5		Olean-12-en-3-ol, acetate, (3.be...	468	C32H52O2	001616-93-9	52



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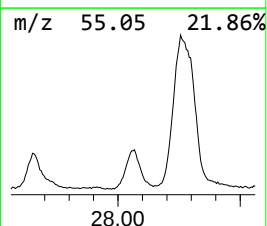
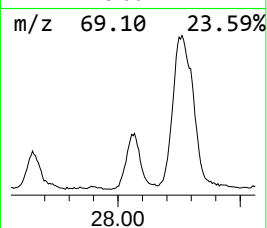
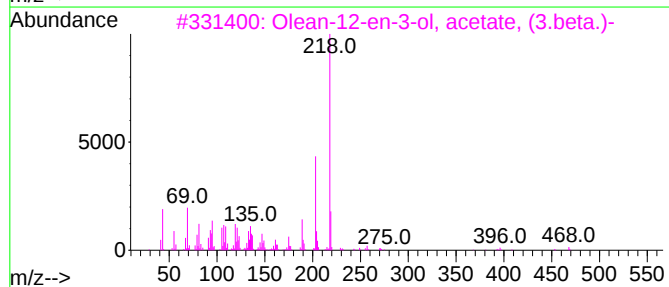
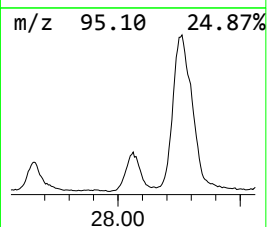
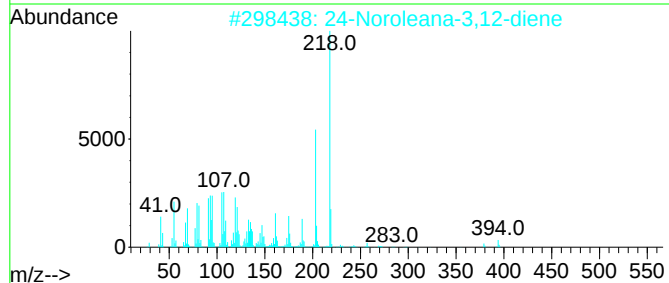
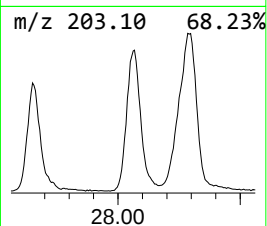
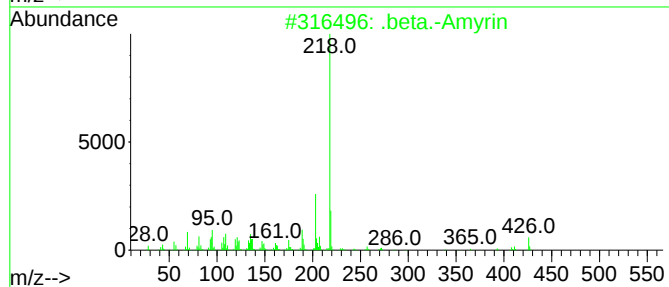
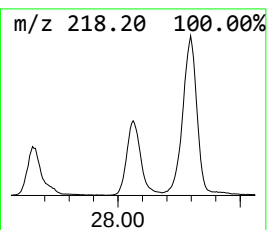
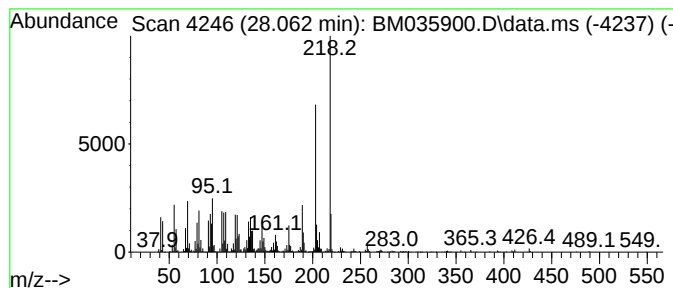
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 .beta.-Amyrin Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.062	16.36 ng	3158050	Perylene-d12	23.815

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Amyrin	426	C30H50O	000559-70-6	97
2		24-Noroleana-3,12-diene	394	C29H46	201358-24-9	94
3		Olean-12-en-3-ol, acetate, (3.beta.)-	468	C32H52O2	001616-93-9	90
4		Pyrene, hexadecahydro-	218	C16H26	002435-85-0	78
5		2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM072122\
Data File : BM035900.D
Acq On : 21 Jul 2022 22:00
Operator : CG/JU
Sample : N3810-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2

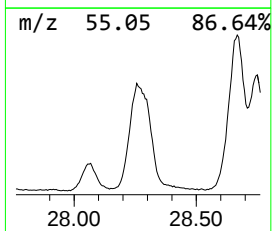
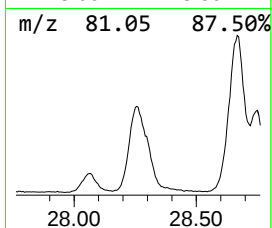
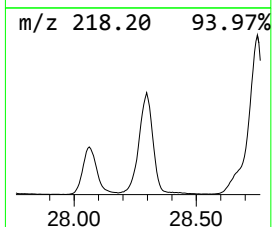
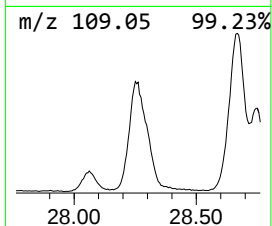
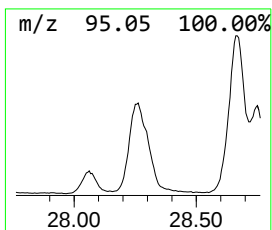
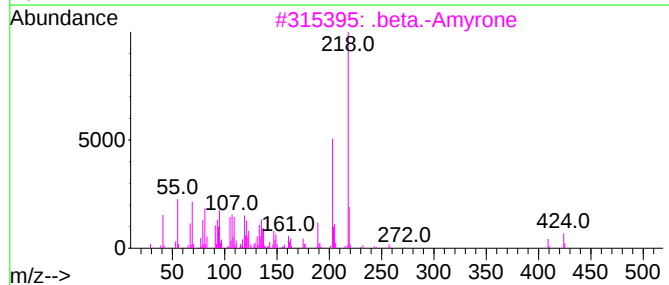
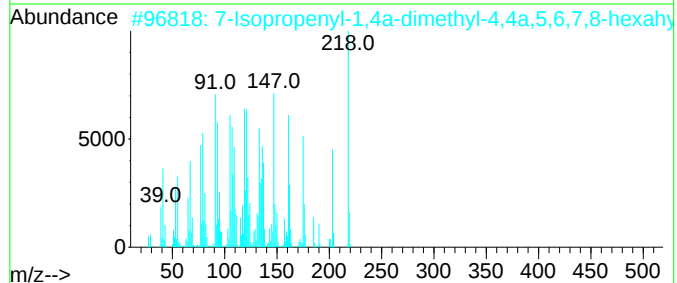
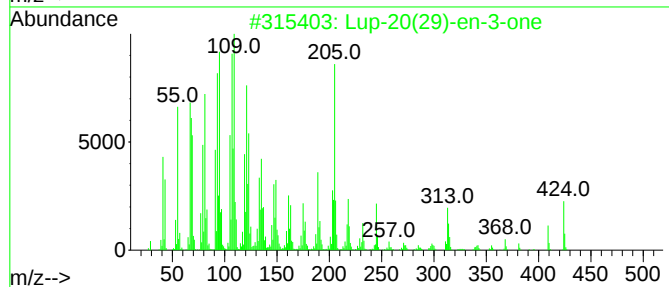
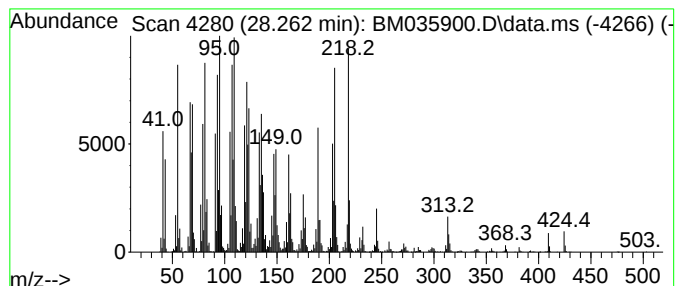
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Lup-20(29)-en-3-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.262	100.65 ng	19435300	Perylene-d12	23.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	99
2			7-Isopropenyl-1,4a-dimethyl-4,4a...	218	C15H22O	000473-08-5	72
3			.beta.-Amyrone	424	C30H48O	000638-97-1	60
4			2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	50
5			13-nor-Eremophil-1(10)-en-11-one	206	C14H22O	054275-21-7	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM072122\
Data File : BM035900.D
Acq On : 21 Jul 2022 22:00
Operator : CG/JU
Sample : N3810-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2

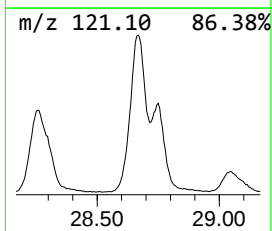
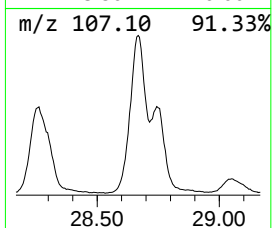
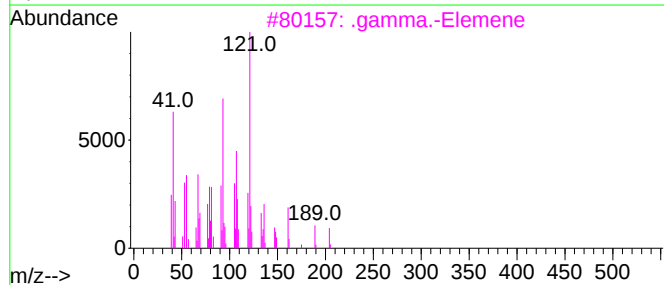
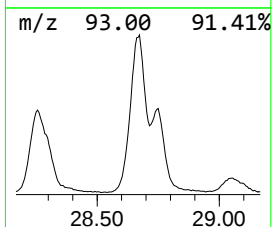
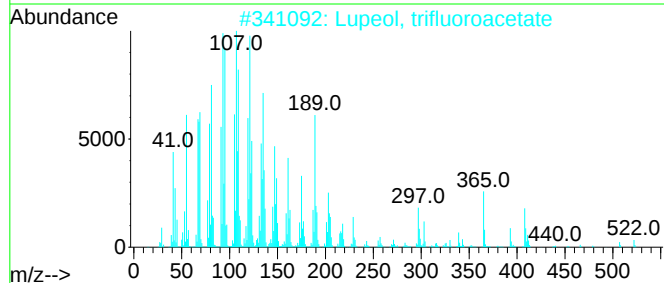
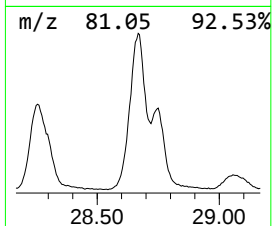
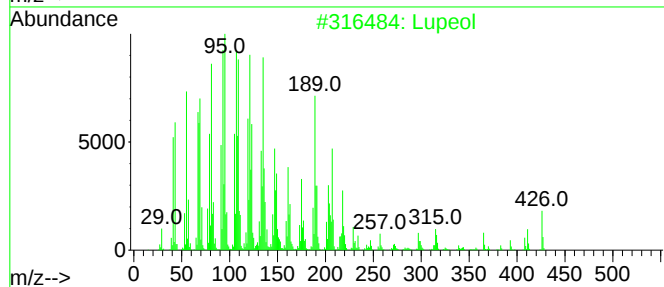
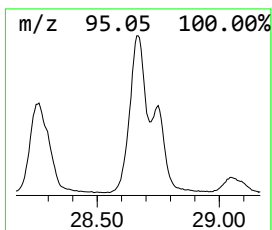
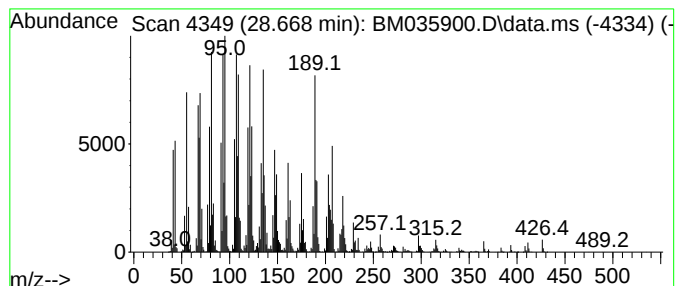
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Lupeol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.668	119.48 ng	23070700	Perylene-d12	23.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lupeol	426	C30H50O	000545-47-1	99
2			Lupeol, trifluoroacetate	522	C32H49F3O2	1000394-56-7	81
3			.gamma.-Elemene	204	C15H24	029873-99-2	60
4			1,5-Cyclodecadiene, 1,5-dimethyl...	204	C15H24	015423-57-1	60
5			Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-3	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM072122\
Data File : BM035900.D
Acq On : 21 Jul 2022 22:00
Operator : CG/JU
Sample : N3810-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2

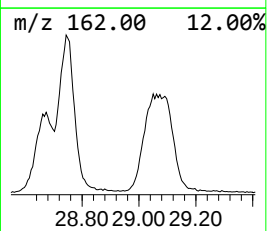
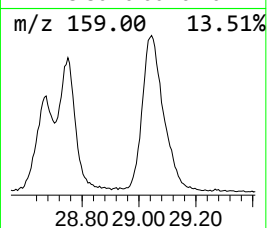
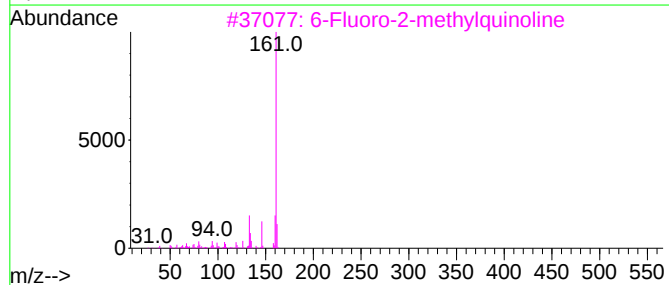
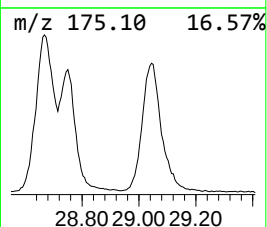
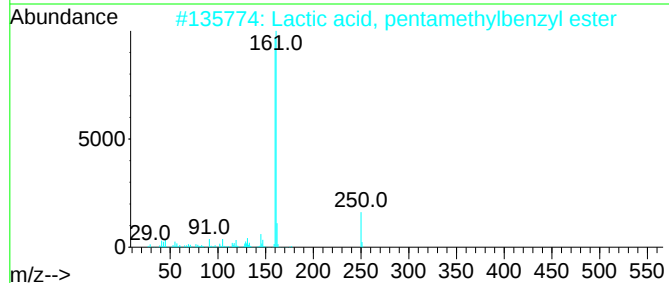
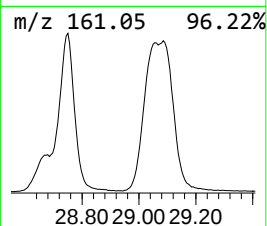
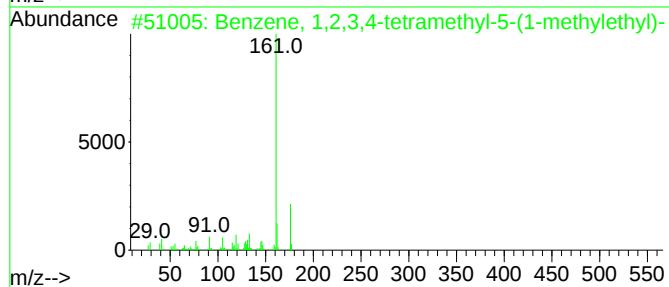
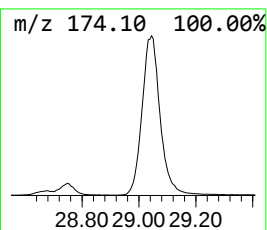
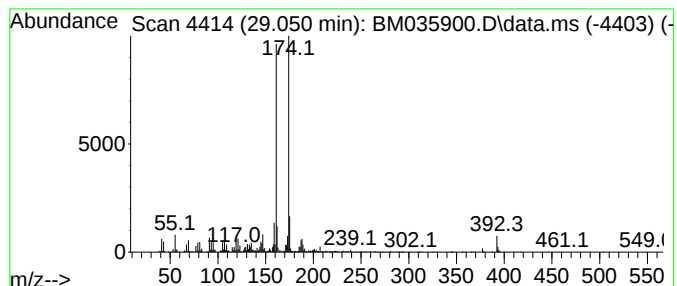
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown29.050 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.050	48.43 ng	9350840	Perylene-d12	23.815

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,2,3,4-tetramethyl-5-(...	176	C13H20	061142-67-4	38
2		Lactic acid, pentamethylbenzyl e...	250	C15H22O3	019405-32-4	35
3		6-Fluoro-2-methylquinoline	161	C10H8FN	001128-61-6	35
4		5-Aminolevulinic acid hexyl este...	359	C17H37N03Si2	1000500-32-9	35
5		1,3,5-Cycloheptatriene, 2,3,4,5,...	176	C13H20	074779-68-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM072122\
Data File : BM035900.D
Acq On : 21 Jul 2022 22:00
Operator : CG/JU
Sample : N3810-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM071822.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
Hexathiane	15.098	3.8	ng	569428	3	14.527	2967580	20.0
Cyclohexadecane	21.162	2.0	ng	468628	5	21.439	4663370	20.0
Benzo[e]pyrene	23.603	2.4	ng	464795	6	23.815	3861820	20.0
Benzene, 1,4-bi...	24.703	6.3	ng	1216210	6	23.815	3861820	20.0
.beta.-Amyrone	27.650	13.1	ng	2531780	6	23.815	3861820	20.0
.beta.-Amyrin	28.062	16.4	ng	3158050	6	23.815	3861820	20.0
Lup-20(29)-en-3...	28.262	100.7	ng	19435300	6	23.815	3861820	20.0
Lupeol	28.668	119.5	ng	23070700	6	23.815	3861820	20.0
unknown29.050	29.050	48.4	ng	9350840	6	23.815	3861820	20.0