

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112822\
 Data File : BF131425.D
 Acq On : 28 Nov 2022 12:28
 Operator : CG\JU
 Sample : N5766-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CR-3

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_F\Methods\8270-BF112122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131425.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.293	24	35	44	rVB	635598	881368	31.43%	4.632%
2	2.405	49	54	60	rVB	37856	46885	1.67%	0.246%
3	5.181	517	526	535	rBV	407412	554712	19.78%	2.915%
4	5.569	586	592	595	rBV	2363228	2310703	82.41%	12.143%
5	6.569	756	762	765	rBV	2131524	2325515	82.94%	12.221%
6	6.951	823	827	830	rBV	653504	526941	18.79%	2.769%
7	7.516	917	923	926	rBV	1561618	1513869	53.99%	7.955%
8	8.239	1041	1046	1049	rBV	779168	681085	24.29%	3.579%
9	9.322	1224	1230	1233	rBV	2982193	2803911	100.00%	14.735%
10	10.004	1341	1346	1350	rBV	962119	797540	28.44%	4.191%
11	10.798	1475	1481	1484	rBV	1984164	1799383	64.17%	9.456%
12	11.504	1597	1601	1604	rBV	913976	800053	28.53%	4.204%
13	13.098	1868	1872	1875	rBV	2787077	2614396	93.24%	13.739%
14	13.998	2021	2025	2043	rBV	106553	217113	7.74%	1.141%
15	14.157	2048	2052	2056	rVB	620288	532286	18.98%	2.797%
16	14.251	2063	2068	2073	rBV	46433	60483	2.16%	0.318%
17	15.033	2198	2201	2205	rBV	47496	51158	1.82%	0.269%
18	15.698	2308	2314	2318	rBV	340266	438628	15.64%	2.305%
19	18.798	2832	2841	2854	rBV	17756	73345	2.62%	0.385%

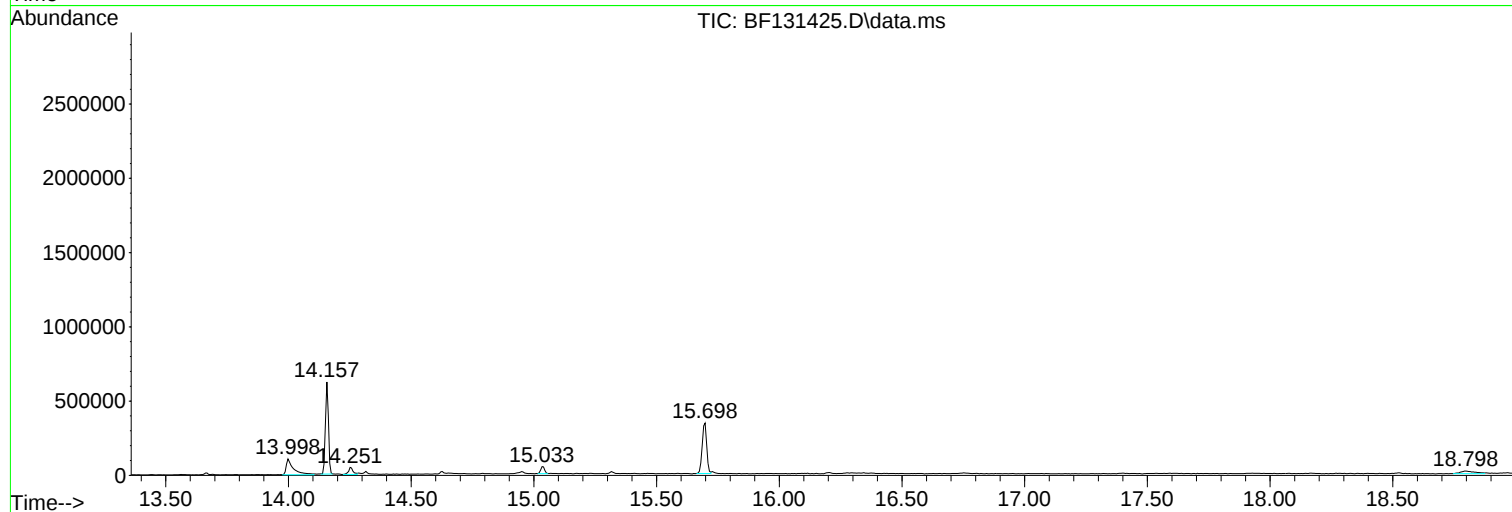
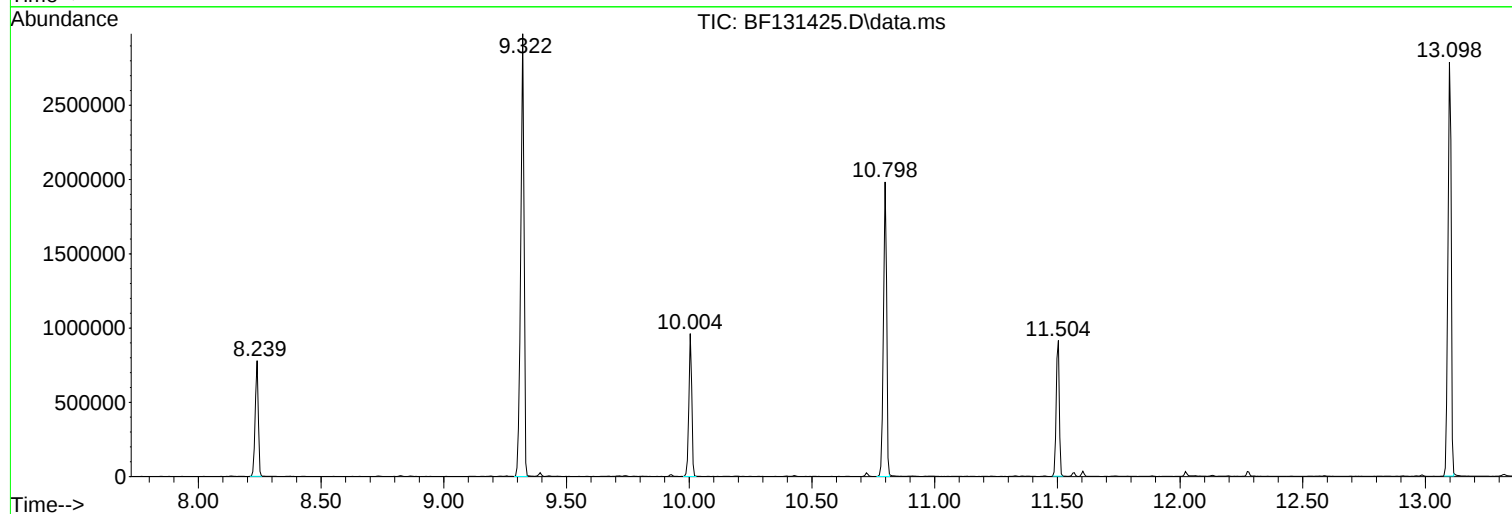
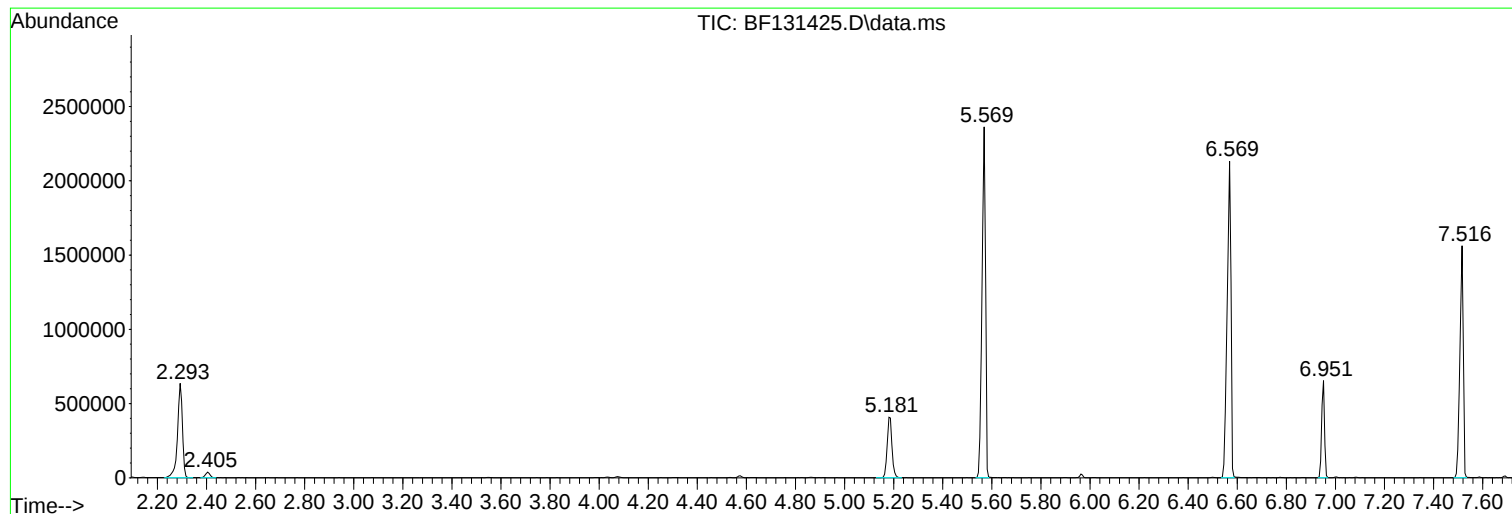
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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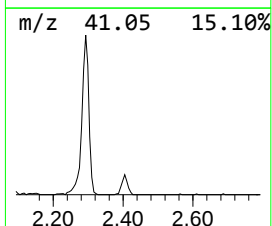
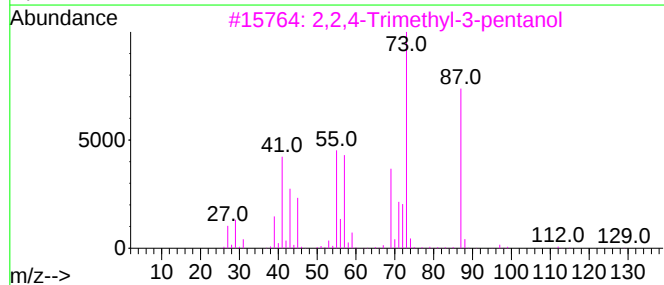
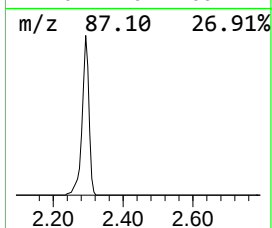
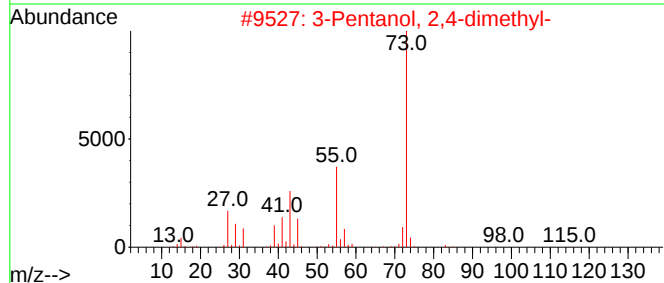
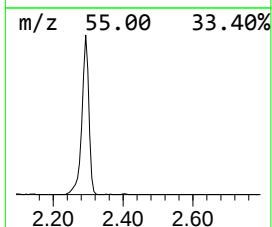
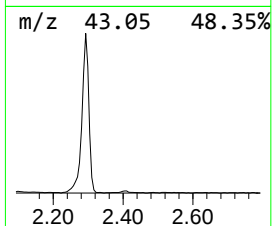
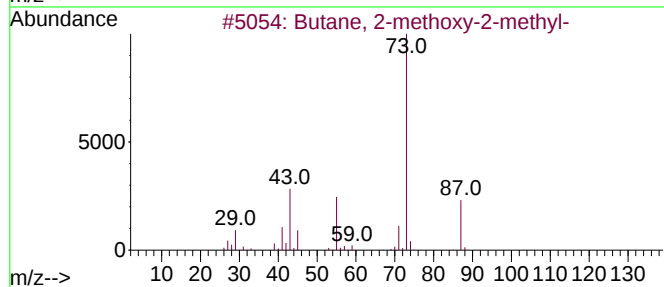
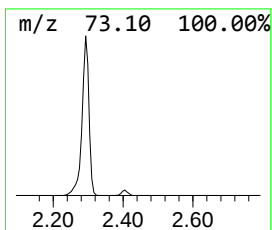
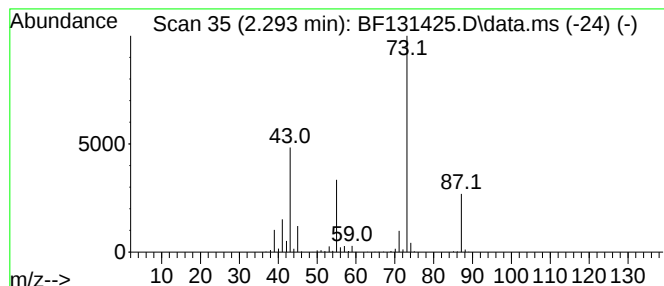
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.293	33.45 ng	881368	1,4-Dichlorobenzene-d4	6.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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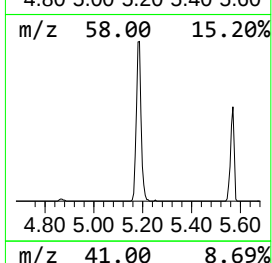
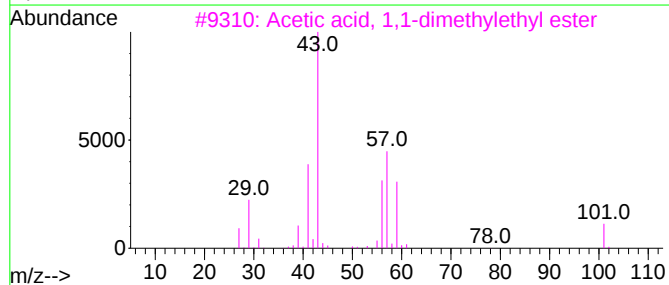
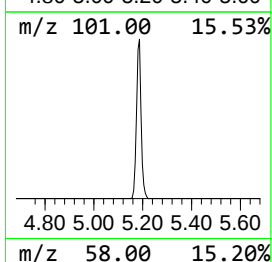
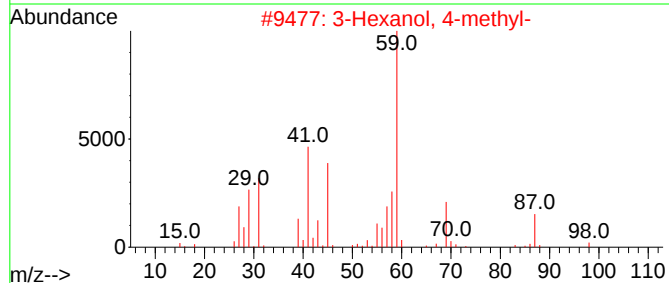
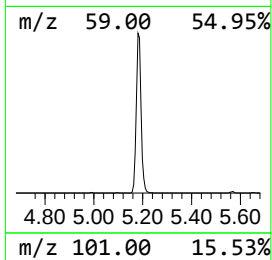
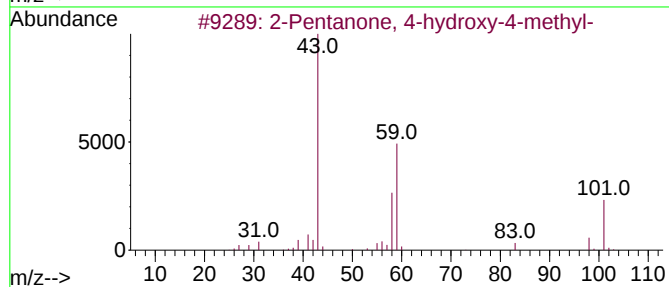
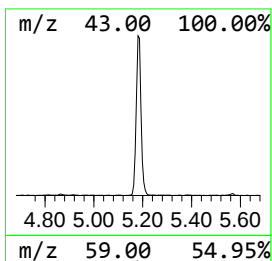
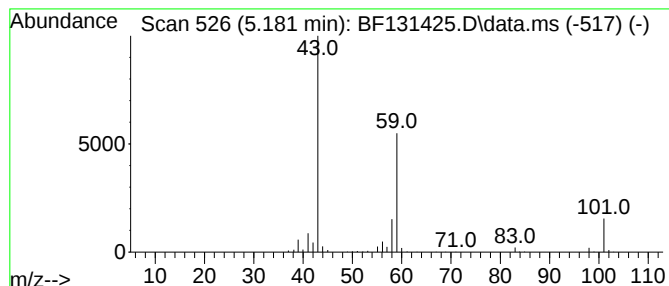
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	21.05 ng	554712	1,4-Dichlorobenzene-d4	6.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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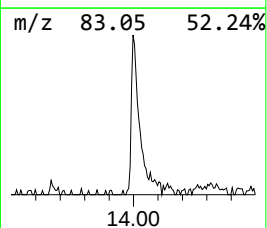
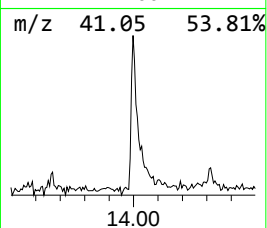
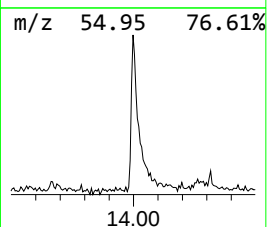
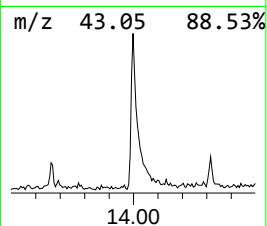
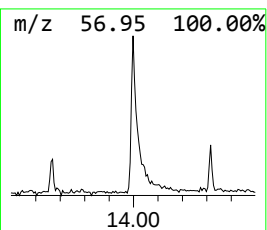
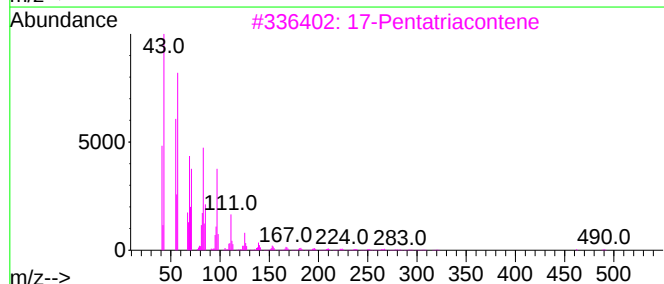
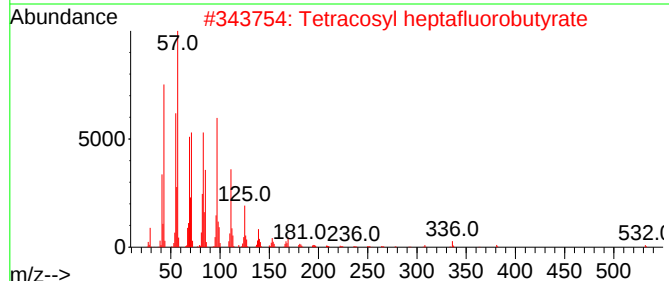
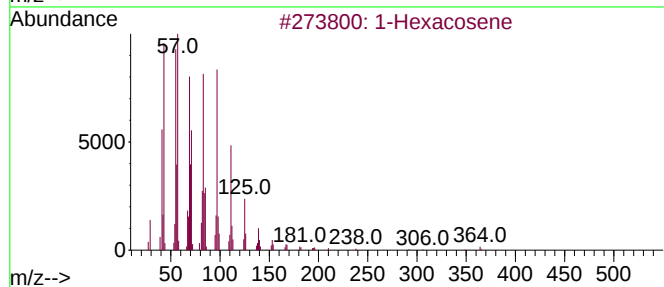
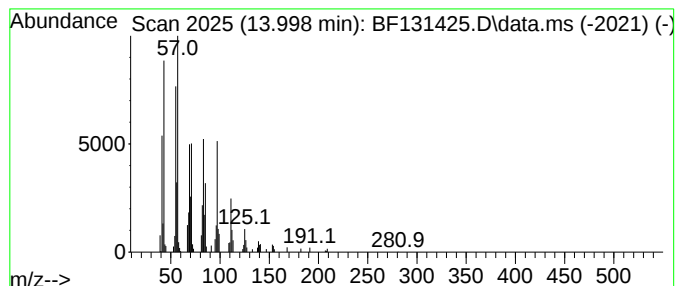
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Peak Number 3 1-Hexacosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	8.16 ng	217113	Chrysene-d12	14.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	91
2	Tetracosyl heptafluorobutyrate			550	C28H49F7O2	1000351-83-7	91
3	17-Pentatriacontene			491	C35H70	006971-40-0	91
4	Octacosyl trifluoroacetate			506	C30H57F3O2	1000351-74-9	91
5	Tricosyl heptafluorobutyrate			536	C27H47F7O2	1000351-83-4	91



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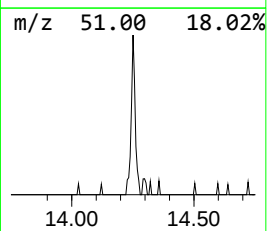
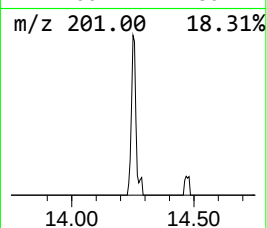
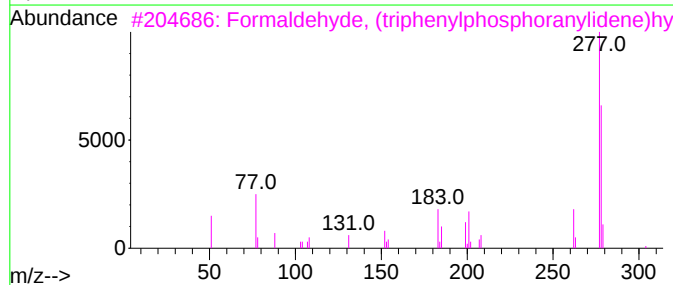
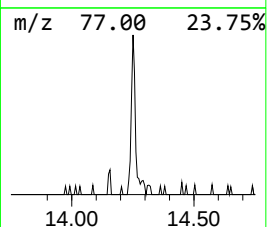
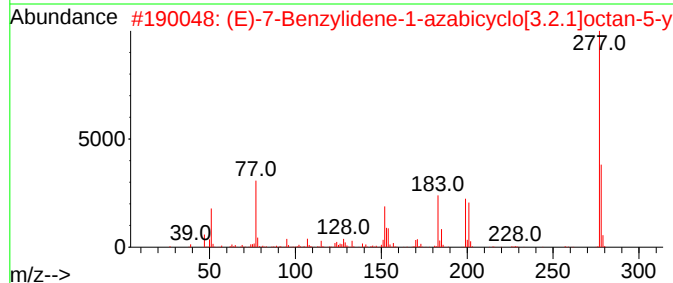
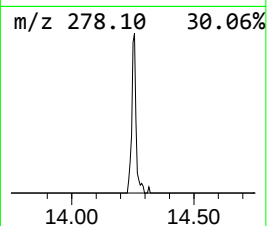
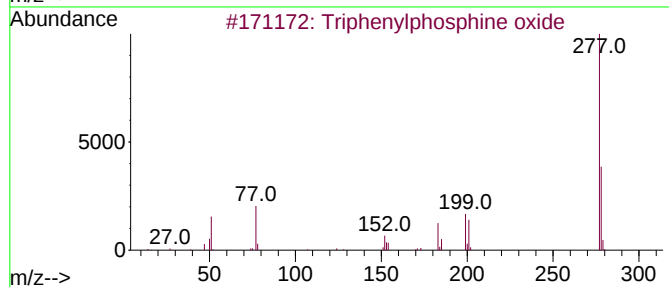
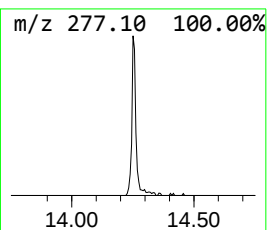
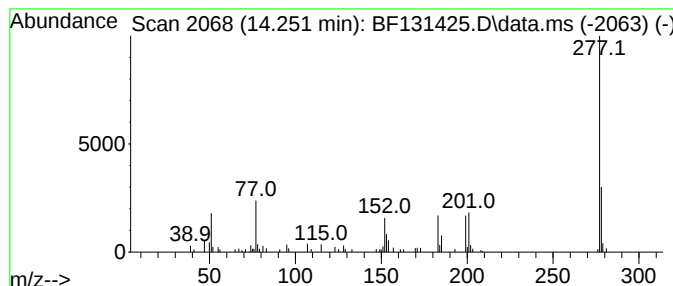
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.251	2.27 ng	60483	Chrysene-d12	14.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	91
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	68
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	64
4			Vanadium, cycloheptatrienyl-(pen...]	277	C17H22V	1000155-20-5	50
5			Cobalt,(.eta.<5>-2,4-cyclopentad...]	277	C16H15BCo	036682-12-9	38



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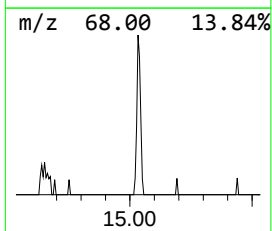
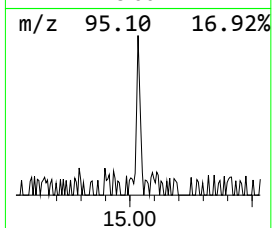
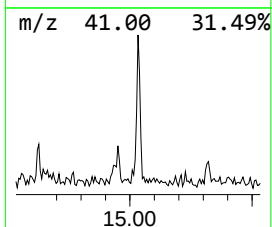
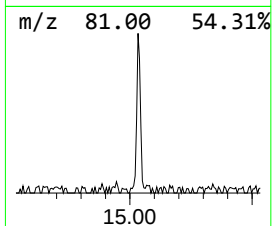
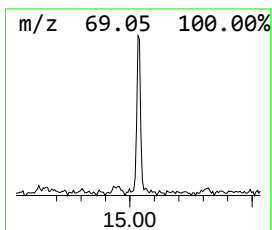
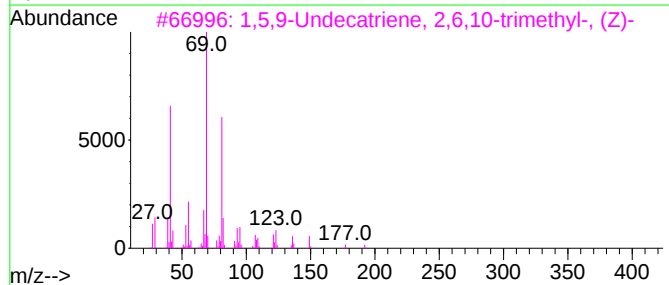
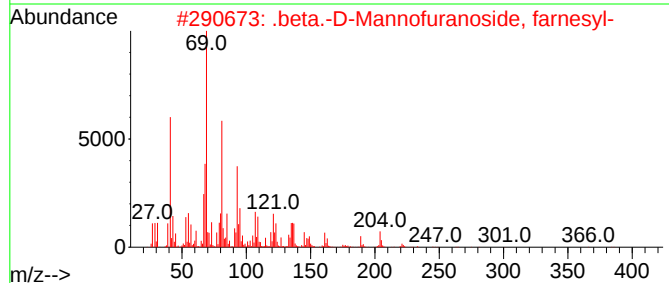
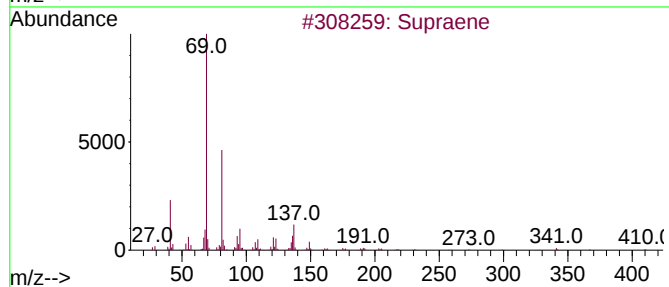
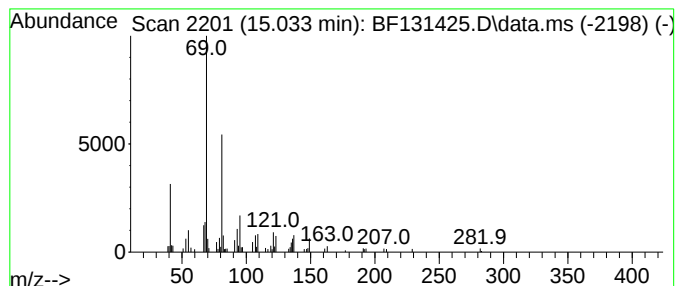
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.033	2.33 ng	51158	Perylene-d12	15.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	86
2			.beta.-D-Mannofuranoside, farnesyl-	384	C21H36O6	1000155-15-5	83
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
5			(2E,6E)-3,7,11-Trimethyldodeca-2...	404	C27H48O2	078368-58-8	72



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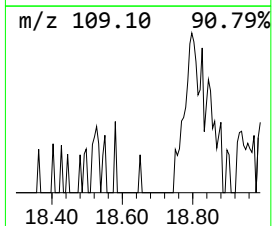
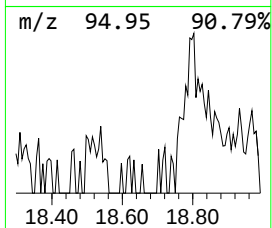
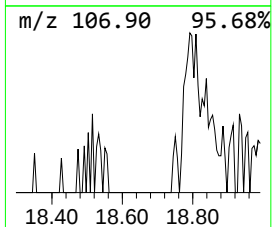
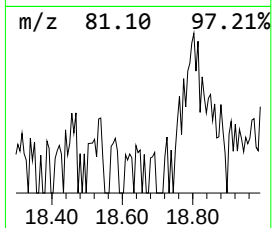
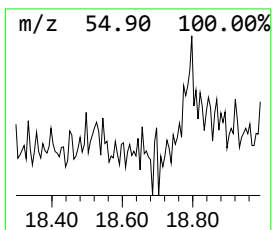
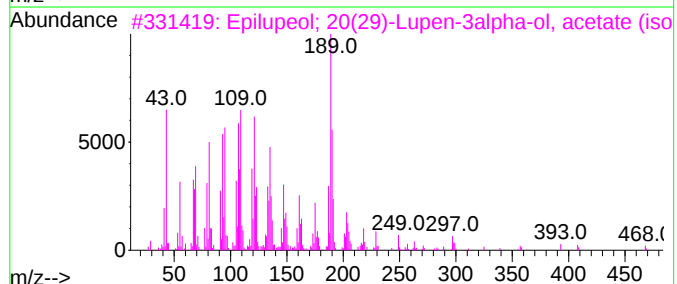
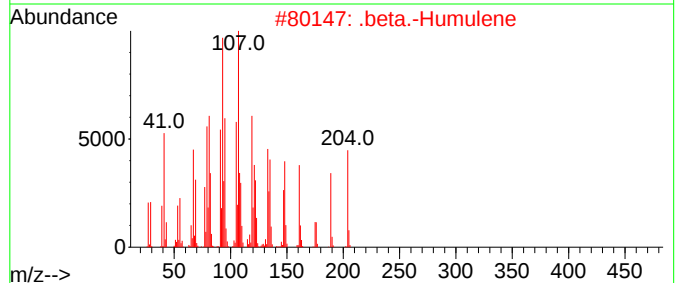
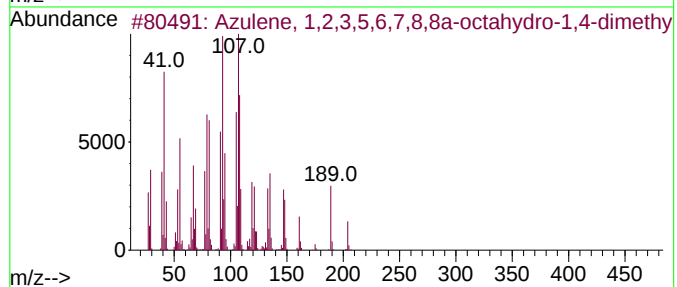
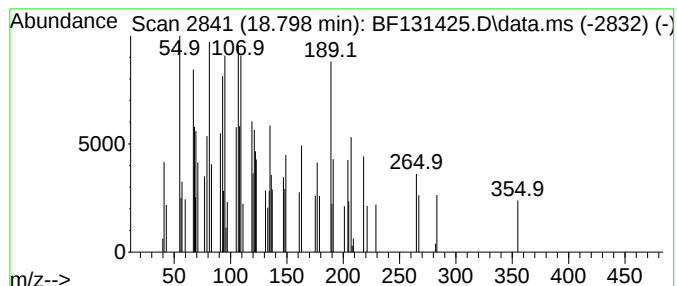
Instrument :
BNA_F
ClientSampleId :
CR-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Azulene, 1,2,3,5,6,7,8,8a-o... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.798	3.34 ng	73345	Perylene-d12	15.698	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	70
2	.beta.-Humulene	204	C15H24	000116-04-1	52
3	Epilupeol; 20(29)-Lupen-3alpha-o...	468	C32H52O2	1010513-01-8	50
4	4,6,6-Trimethyl-2-(3-methylbuta-...	218	C15H22O	1000190-22-2	46
5	(1S,4aR,7R)-1,4a-Dimethyl-7-(pro...	204	C15H24	052026-55-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112822\
Data File : BF131425.D
Acq On : 28 Nov 2022 12:28
Operator : CG\JU
Sample : N5766-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CR-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
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...	2.293	33.5	ng	881368	1	6.951	526941	20.0
2-Pentanone, 4-...	5.181	21.1	ng	554712	1	6.951	526941	20.0
1-Hexacosene	13.998	8.2	ng	217113	5	14.157	532286	20.0
Triphenylphosph...	14.251	2.3	ng	60483	5	14.157	532286	20.0
Supraene	15.033	2.3	ng	51158	6	15.698	438628	20.0
Azulene, 1,2,3,...	18.798	3.3	ng	73345	6	15.698	438628	20.0