

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
 Data File : BF131783.D
 Acq On : 22 Dec 2022 18:33
 Operator : CG\JU
 Sample : N6178-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-1

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-BF122022.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131783.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	13	rVB	435136	527090	17.70%	2.668%
2	5.069	501	507	517	rVB	705419	934874	31.39%	4.733%
3	5.469	571	575	578	rBV	2248550	2224696	74.69%	11.263%
4	6.487	743	748	751	rBV	2267824	2257399	75.79%	11.428%
5	6.851	807	810	814	rBV	640112	490722	16.48%	2.484%
6	7.422	902	907	910	rBV	1521113	1482623	49.78%	7.506%
7	8.145	1025	1030	1033	rBV	648348	617216	20.72%	3.125%
8	9.222	1208	1213	1216	rBV	2866864	2788348	93.62%	14.116%
9	9.533	1262	1266	1268	rBV	91624	77901	2.62%	0.394%
10	9.904	1325	1329	1332	rBV	910535	748984	25.15%	3.792%
11	10.622	1446	1451	1454	rBV	87156	68039	2.28%	0.344%
12	10.698	1459	1464	1467	rBV	2289535	1923152	64.57%	9.736%
13	11.398	1579	1583	1586	rBV	960345	818638	27.49%	4.144%
14	11.922	1669	1672	1677	rBV	139131	126565	4.25%	0.641%
15	12.474	1762	1766	1768	rBV	147206	125440	4.21%	0.635%
16	12.492	1768	1769	1777	rVB2	72949	63412	2.13%	0.321%
17	12.992	1849	1854	1857	rBV	3170535	2978482	100.00%	15.079%
18	13.416	1923	1926	1929	rBV	61297	52013	1.75%	0.263%
19	13.886	2002	2006	2027	rBV2	90848	293129	9.84%	1.484%
20	14.045	2029	2033	2036	rVV	739798	618191	20.76%	3.130%
21	14.139	2045	2049	2054	rBV	68030	66568	2.23%	0.337%
22	15.533	2280	2286	2294	rBV	346018	437861	14.70%	2.217%
23	15.998	2360	2365	2371	rVB3	20407	31588	1.06%	0.160%

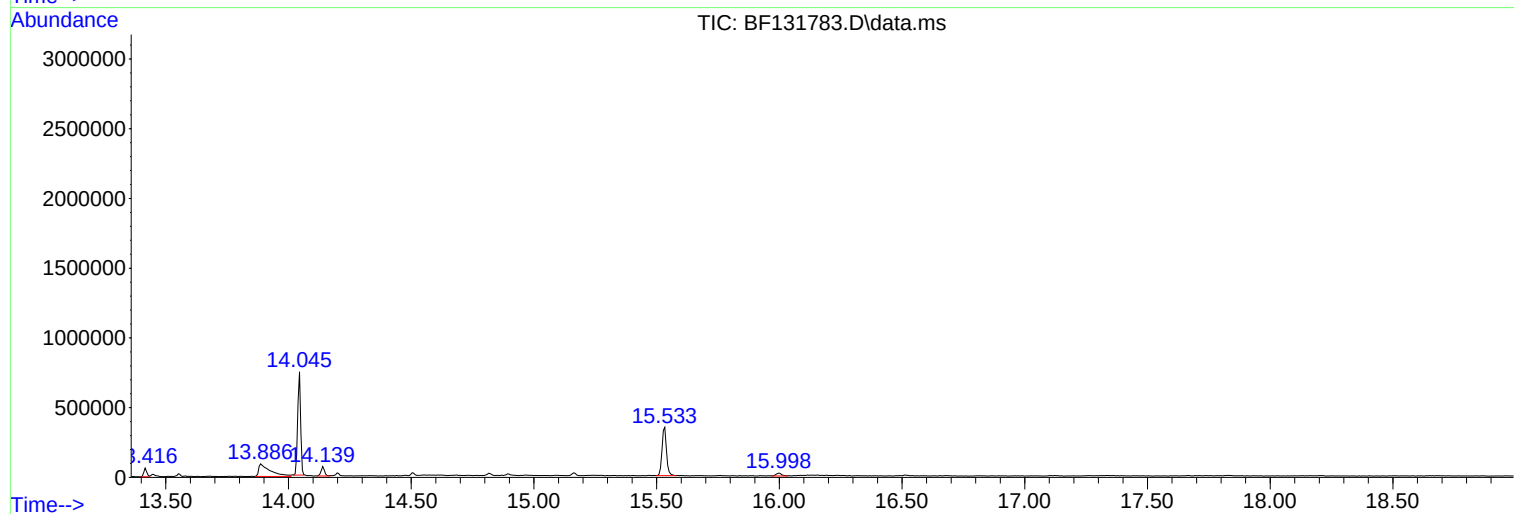
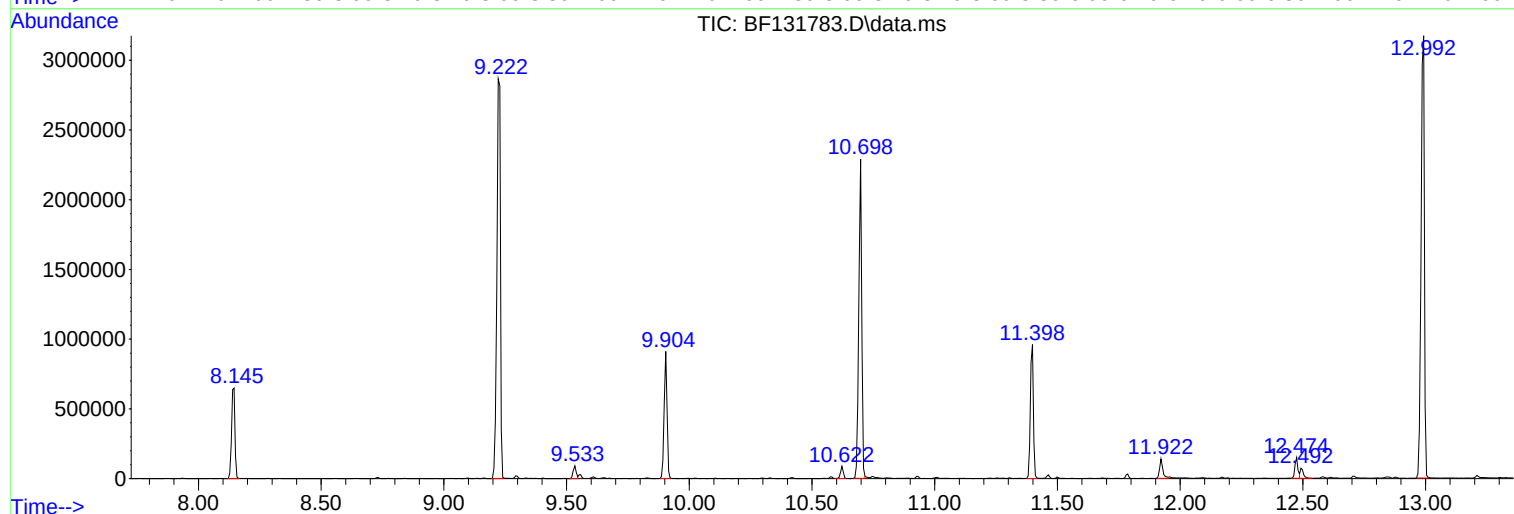
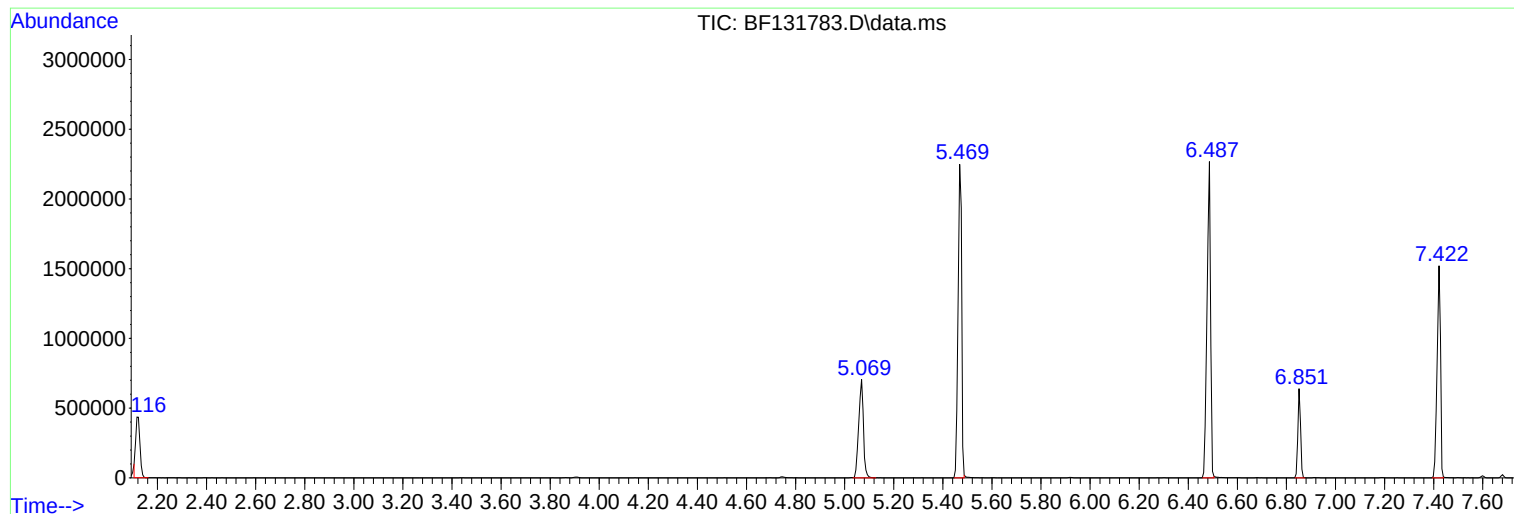
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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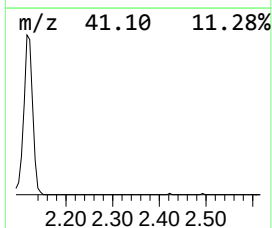
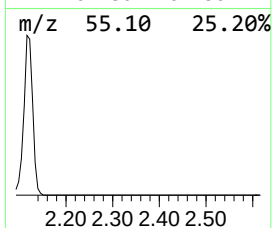
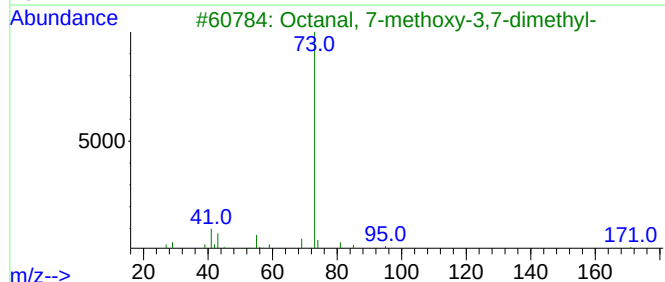
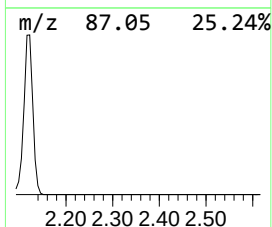
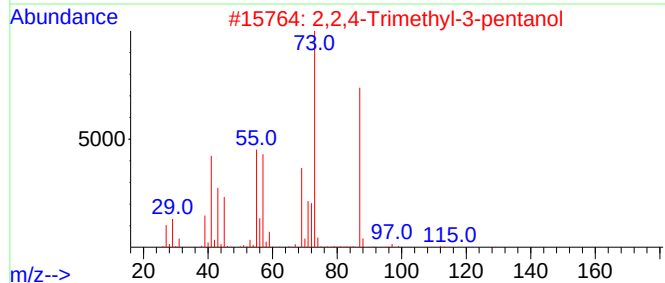
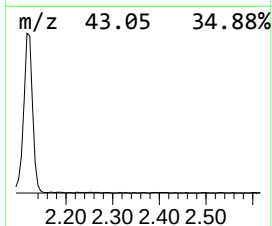
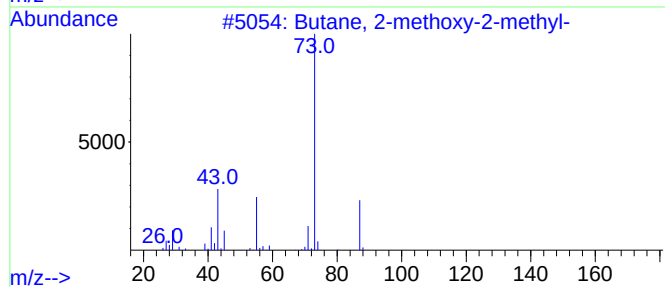
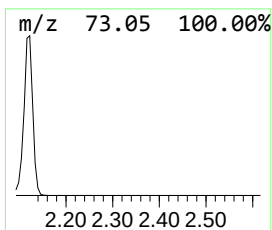
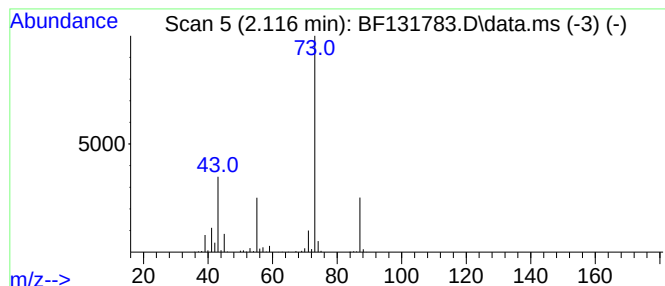
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	21.48 ng	527090	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	23
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22



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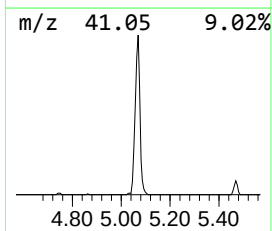
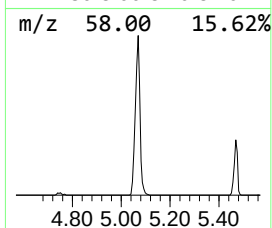
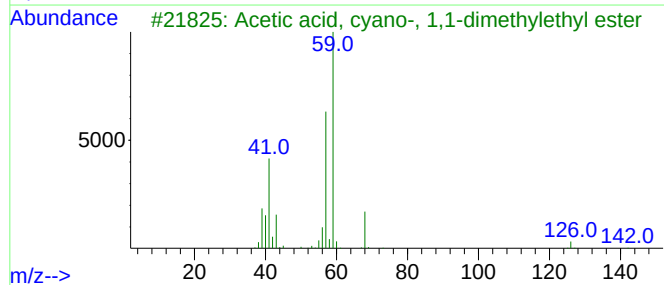
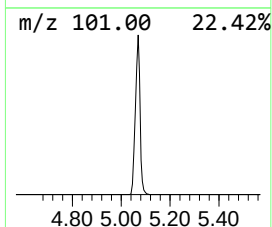
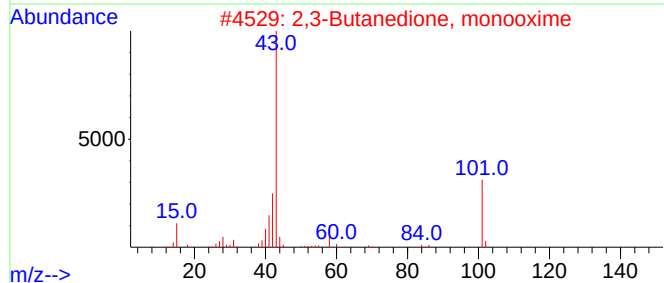
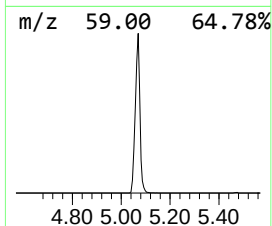
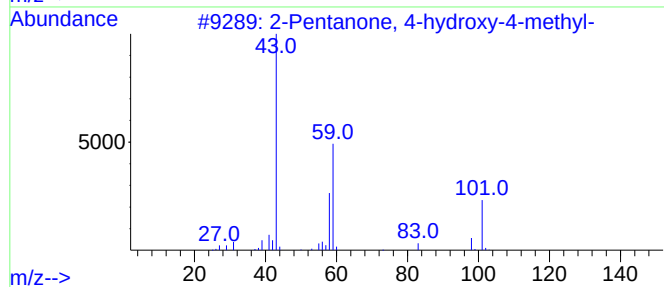
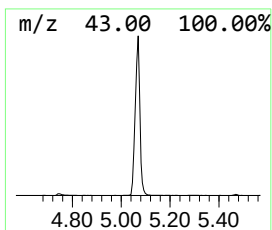
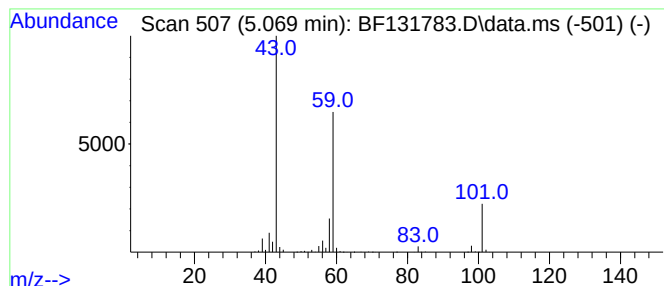
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	38.10 ng	934874	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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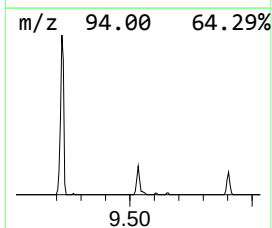
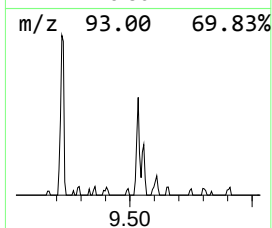
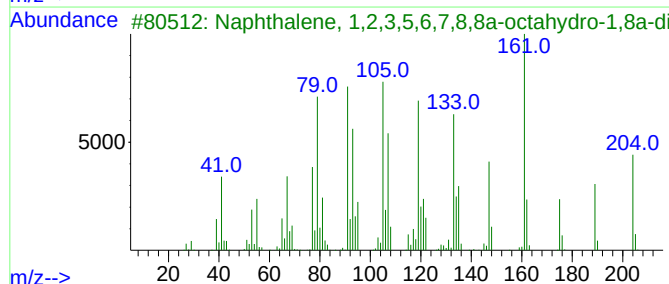
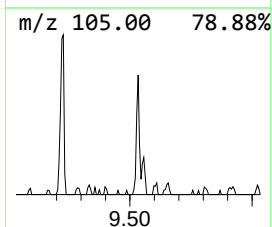
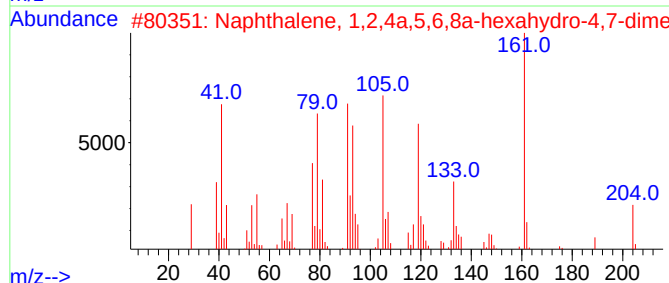
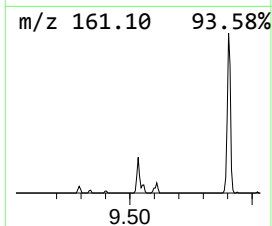
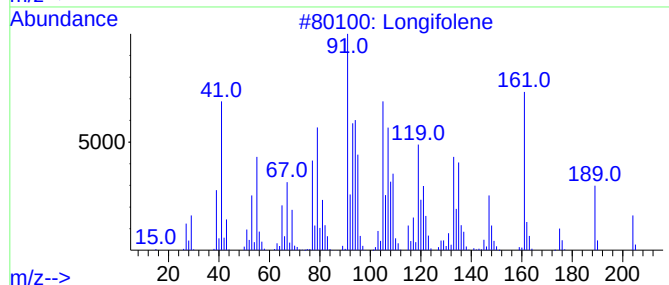
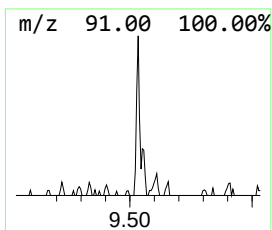
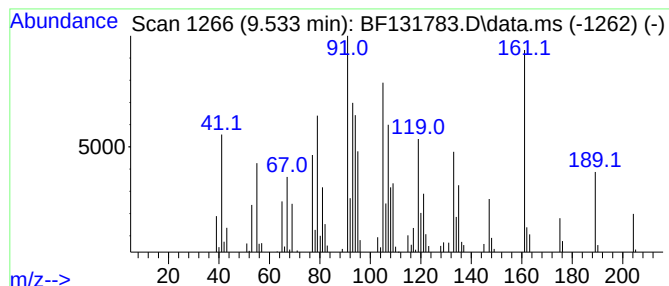
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Peak Number 3 Longifolene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.533	2.08 ng	77901	Acenaphthene-d10	9.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Longifolene	204	C15H24	000475-20-7	99
2			Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	95
3			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	91
4			Aromandendrene	204	C15H24	000489-39-4	90
5			1H-Cycloprop[e]azulene, decahydr...	204	C15H24	072747-25-2	90



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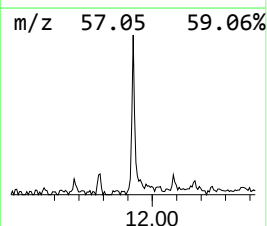
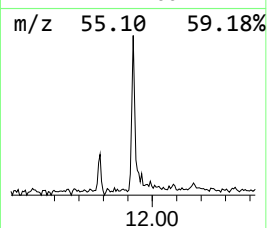
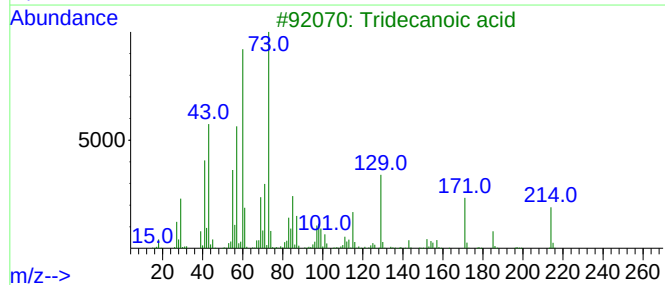
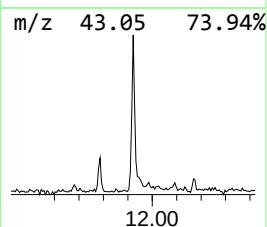
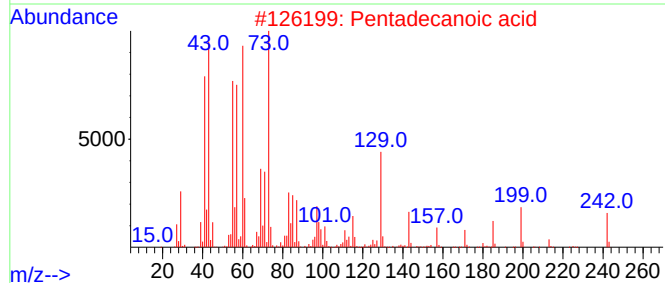
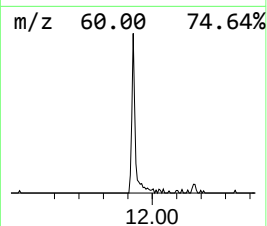
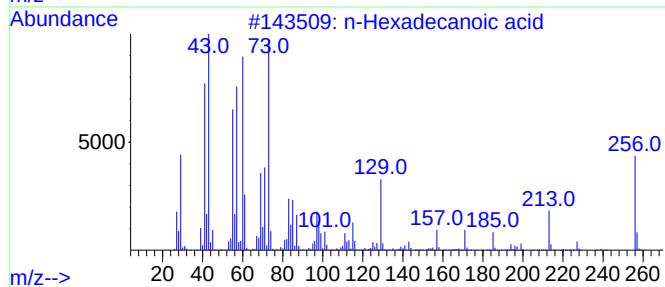
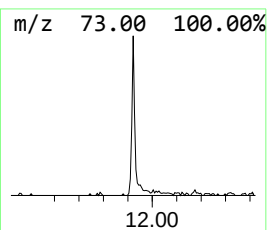
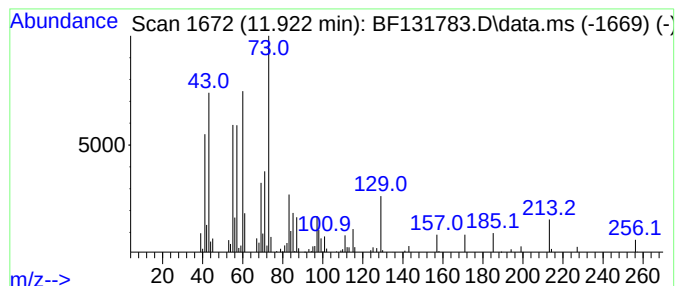
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.09 ng	126565	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3			Tridecanoic acid	214	C13H26O2	000638-53-9	86
4			Undecanoic acid	186	C11H22O2	000112-37-8	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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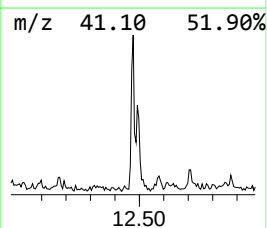
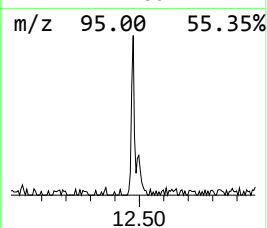
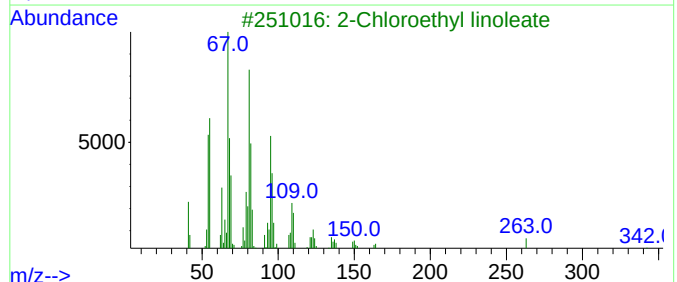
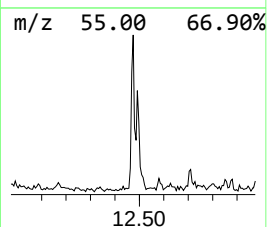
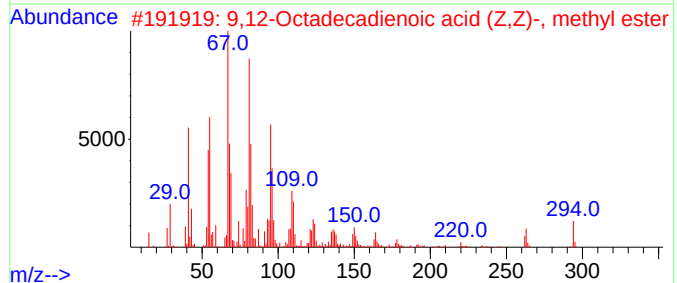
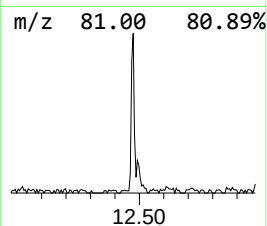
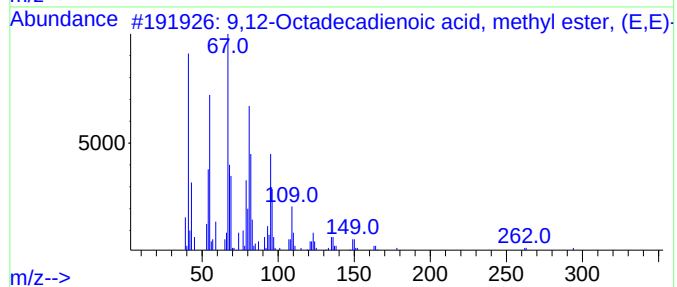
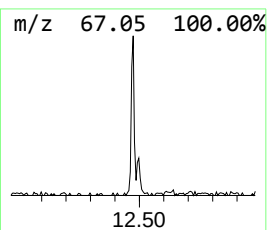
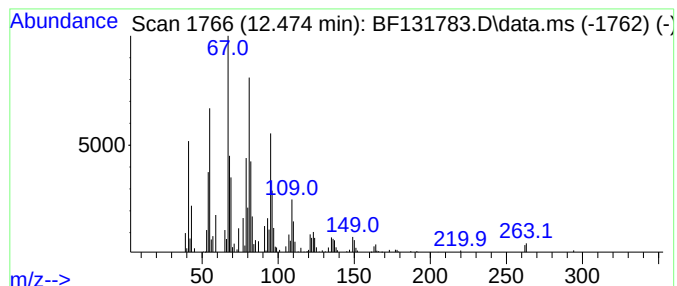
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.475	3.06 ng	125440	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95
3			2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	93
4			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	93
5			Linoelaidic acid	280	C18H32O2	000506-21-8	91



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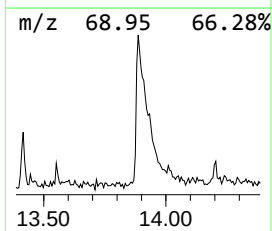
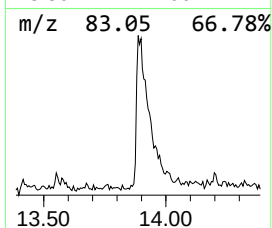
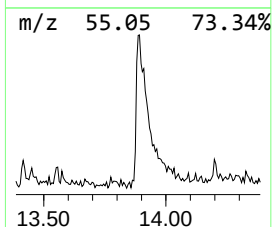
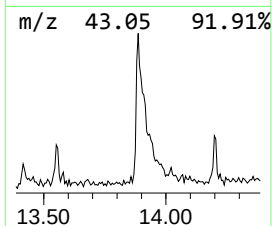
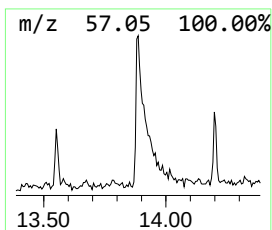
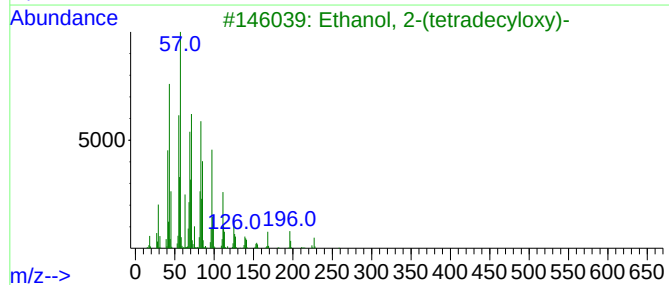
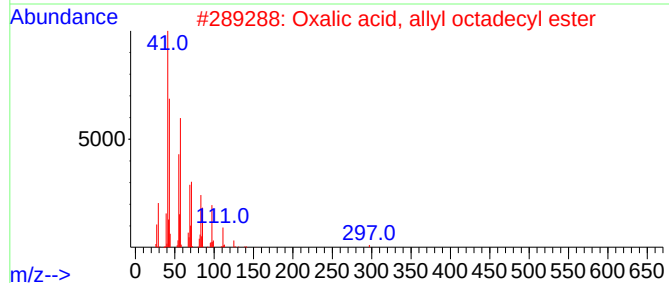
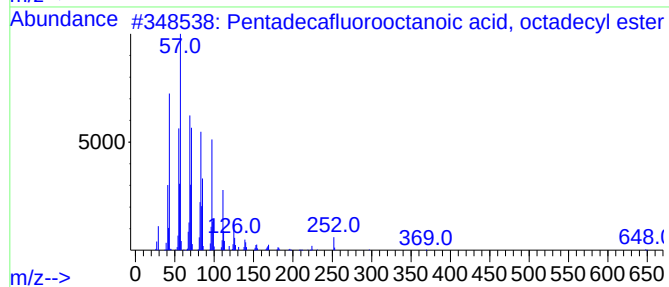
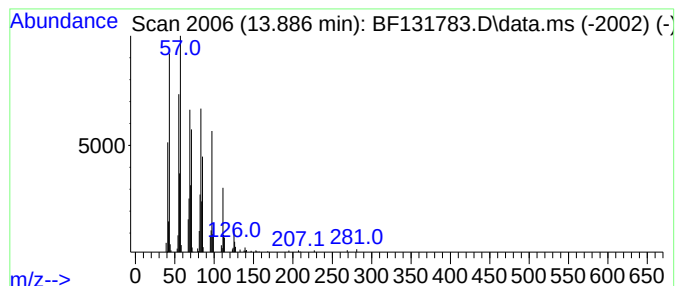
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	9.48 ng	293129	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
2			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	87
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	81
5			1-Hexacosene	364	C26H52	018835-33-1	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
Data File : BF131783.D
Acq On : 22 Dec 2022 18:33
Operator : CG\JU
Sample : N6178-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

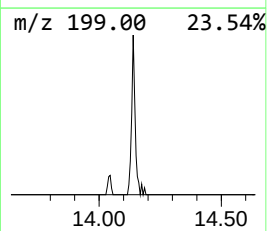
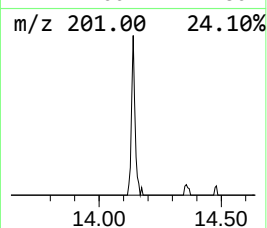
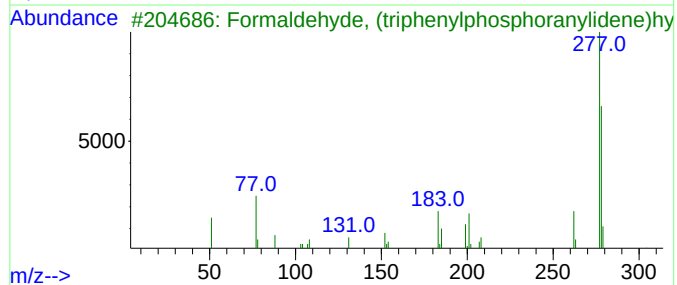
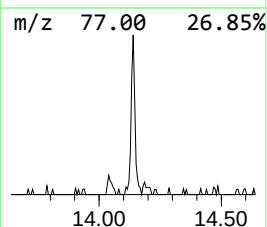
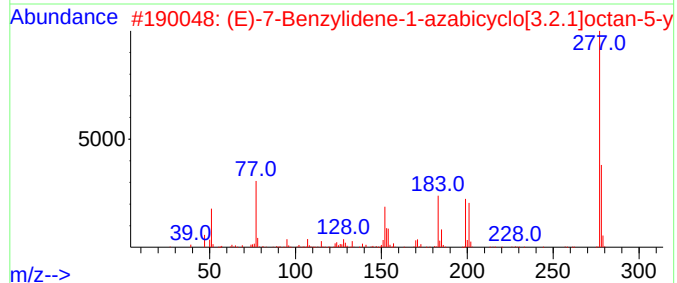
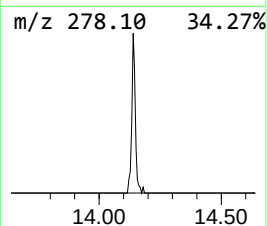
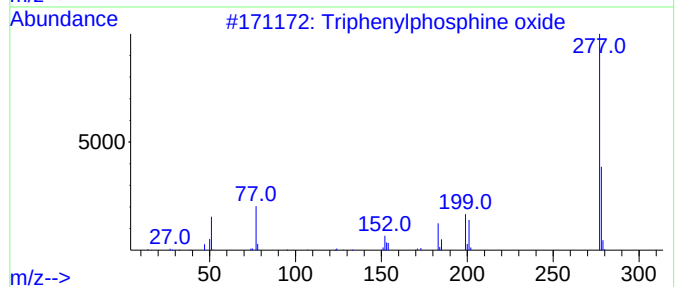
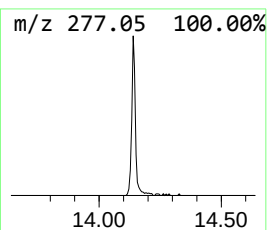
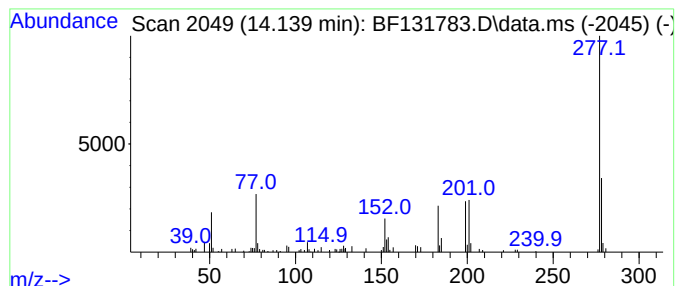
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.139	2.15 ng	66568	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	62
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	28
5			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122222\
Data File : BF131783.D
Acq On : 22 Dec 2022 18:33
Operator : CG\JU
Sample : N6178-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.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...	2.116	21.5	ng	527090	1	6.851	490722	20.0
2-Pentanone, 4-...	5.069	38.1	ng	934874	1	6.851	490722	20.0
Longifolene	9.533	2.1	ng	77901	3	9.904	748984	20.0
n-Hexadecanoic ...	11.922	3.1	ng	126565	4	11.398	818638	20.0
9,12-Octadecadi...	12.475	3.1	ng	125440	4	11.398	818638	20.0
Pentadecafluoro...	13.886	9.5	ng	293129	5	14.045	618191	20.0
Triphenylphosph...	14.139	2.1	ng	66568	5	14.045	618191	20.0