

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010522\
 Data File : BF126504.D
 Acq On : 5 Jan 2022 19:13
 Operator : JU/CG
 Sample : M5196-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-SAMPLE-1-DEEP

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-BF122921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126504.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.158	8	12	16	rVB	39055	48643	2.06%	0.282%
2	4.993	490	494	502	rVB	68303	82860	3.51%	0.480%
3	5.399	558	563	566	rBV	2432269	2278933	96.45%	13.210%
4	6.416	731	736	739	rBV	2335257	2362912	100.00%	13.697%
5	6.781	794	798	801	rBV	690247	548131	23.20%	3.177%
6	7.345	888	894	897	rBV	1574155	1548392	65.53%	8.975%
7	8.063	1012	1016	1019	rBV	935929	762763	32.28%	4.421%
8	9.139	1194	1199	1203	rBV	2369882	2323252	98.32%	13.467%
9	9.228	1210	1214	1219	rVB	42099	33451	1.42%	0.194%
10	9.816	1310	1314	1318	rBV	888948	789288	33.40%	4.575%
11	10.604	1444	1448	1452	rBV	1359844	1336288	56.55%	7.746%
12	11.304	1563	1567	1570	rBV	919868	758823	32.11%	4.398%
13	11.704	1631	1635	1638	rVB	60697	43930	1.86%	0.255%
14	11.839	1655	1658	1661	rBV	114500	114132	4.83%	0.662%
15	12.410	1752	1755	1758	rVB	92878	70102	2.97%	0.406%
16	12.622	1788	1791	1796	rBV2	51903	57200	2.42%	0.332%
17	12.774	1813	1817	1829	rVB	40383	63824	2.70%	0.370%
18	12.892	1833	1837	1840	rBV	2248010	2101313	88.93%	12.180%
19	13.792	1986	1990	1999	rBV2	182300	287423	12.16%	1.666%
20	13.939	2011	2015	2019	rVB	701535	599116	25.35%	3.473%
21	14.039	2022	2032	2040	rBV	143210	169067	7.16%	0.980%
22	14.421	2094	2097	2105	rBV4	24467	55279	2.34%	0.320%
23	14.698	2141	2144	2152	rBV2	90151	102217	4.33%	0.592%
24	14.804	2157	2162	2166	rVB	161850	167440	7.09%	0.971%
25	15.380	2254	2260	2264	rBV	398407	483120	20.45%	2.800%
26	15.839	2334	2338	2344	rVB4	16837	24497	1.04%	0.142%
27	15.904	2344	2349	2355	rBV7	14422	39518	1.67%	0.229%

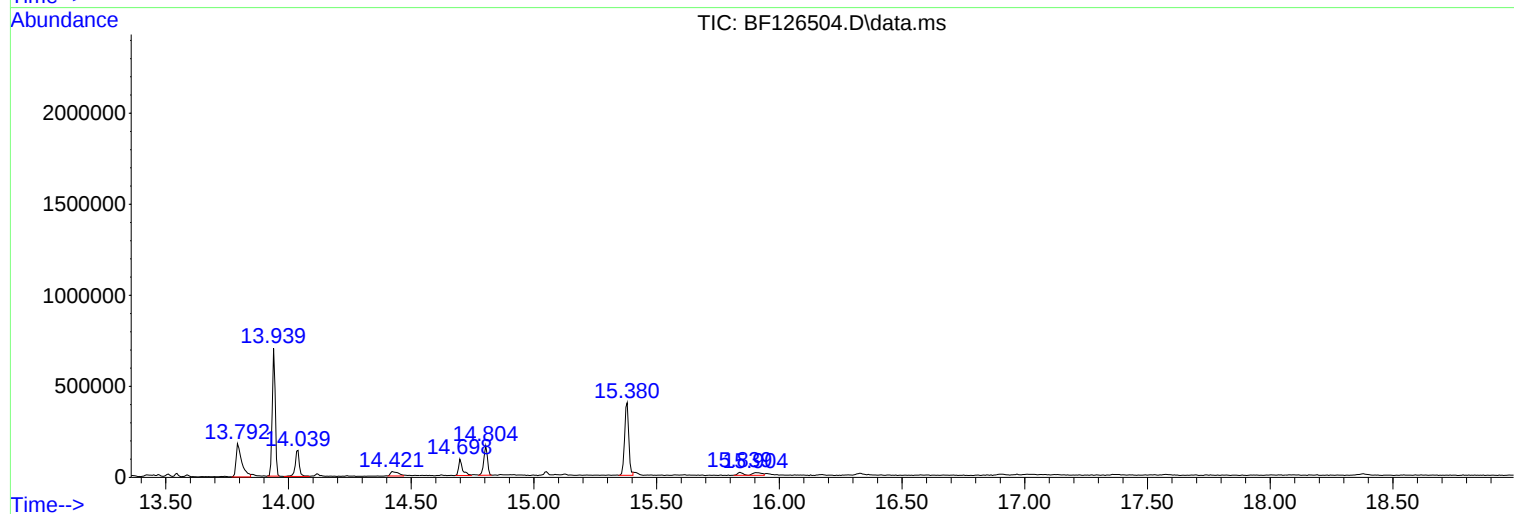
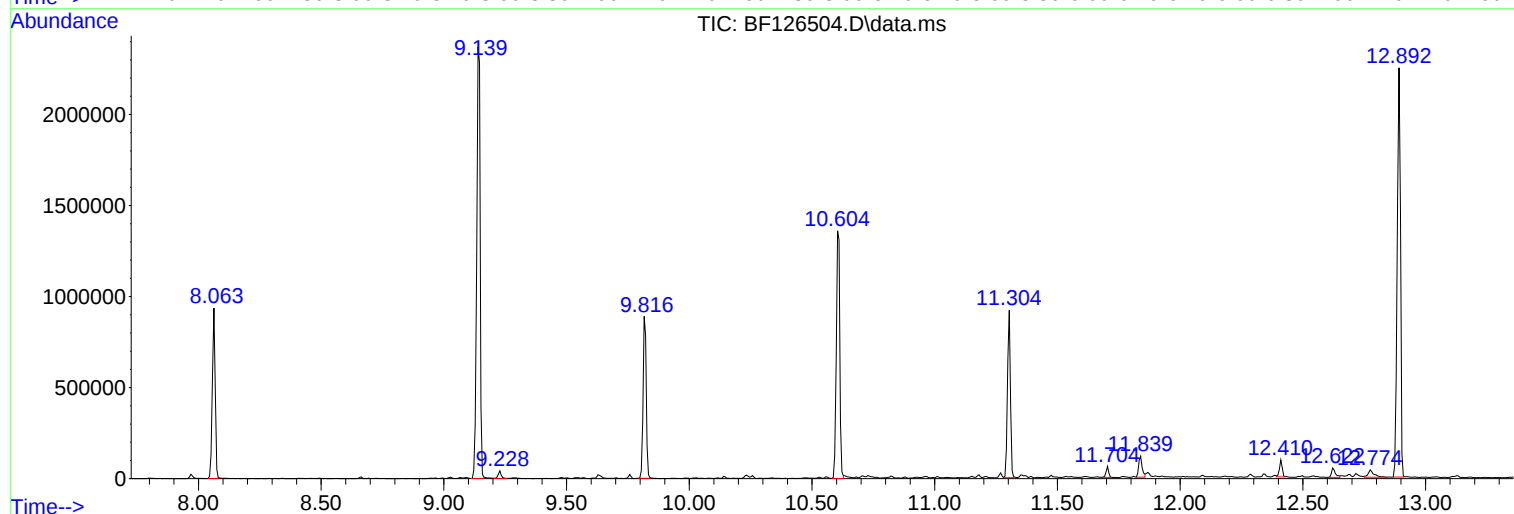
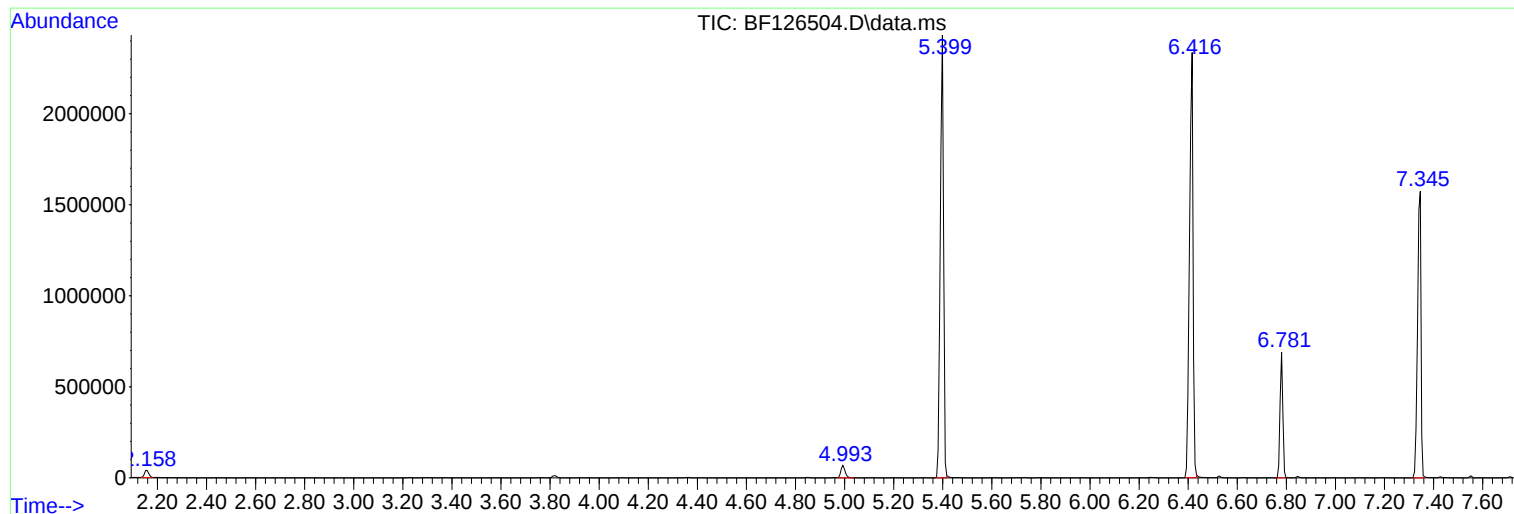
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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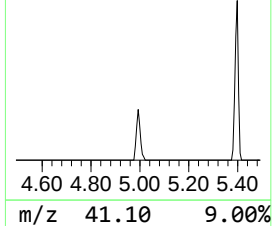
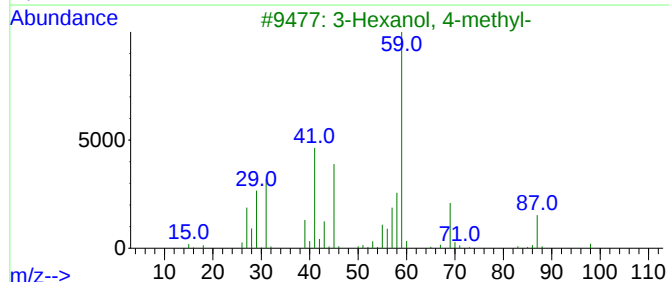
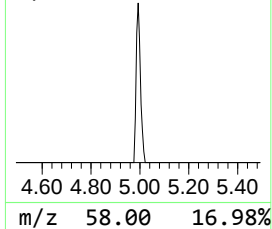
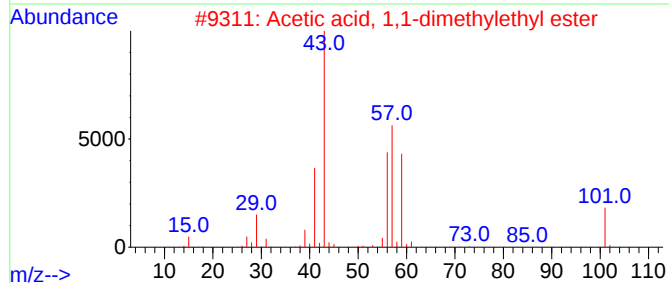
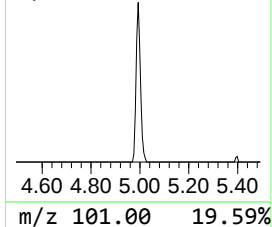
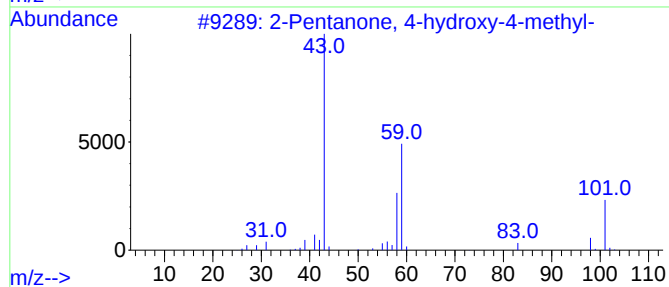
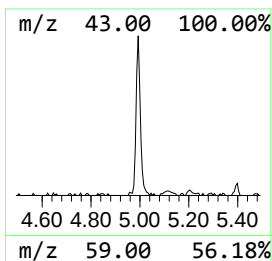
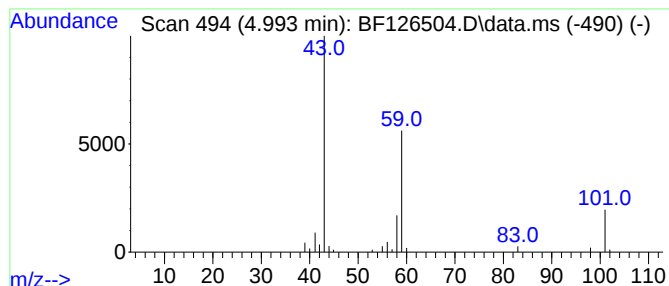
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.993	3.02 ng	82860	1,4-Dichlorobenzene-d4	6.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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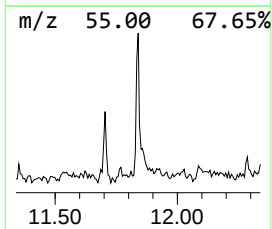
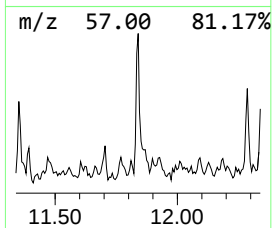
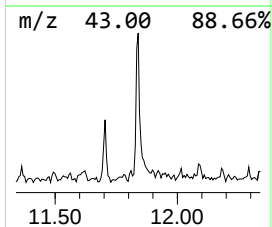
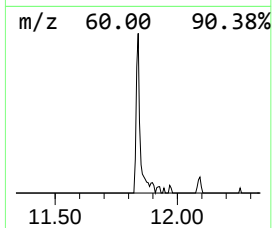
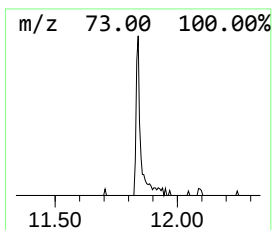
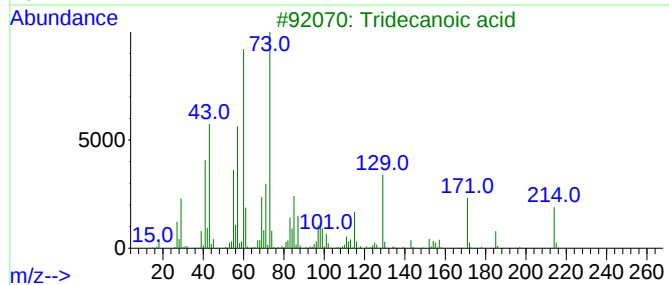
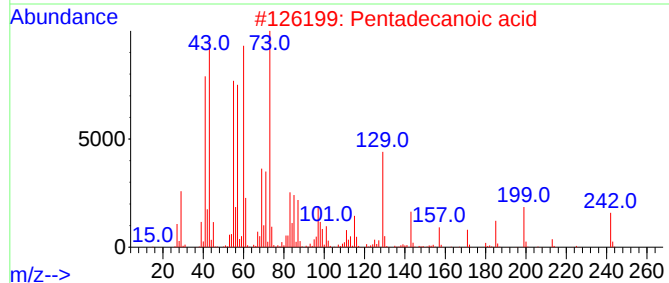
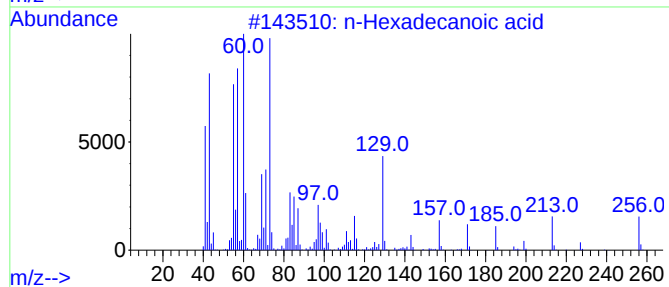
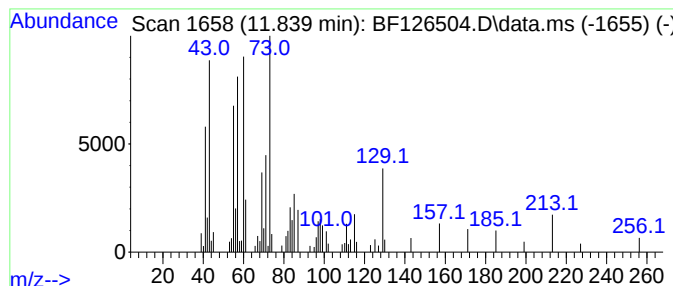
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	3.01 ng	114132	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Dodecanoic acid	200	C12H24O2	000143-07-7	72



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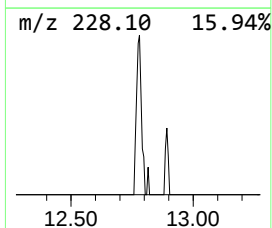
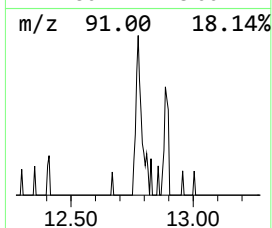
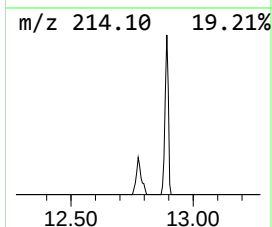
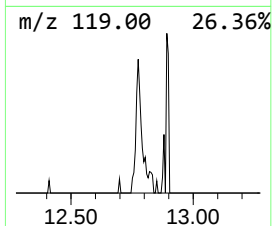
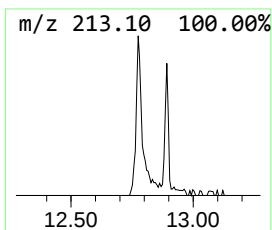
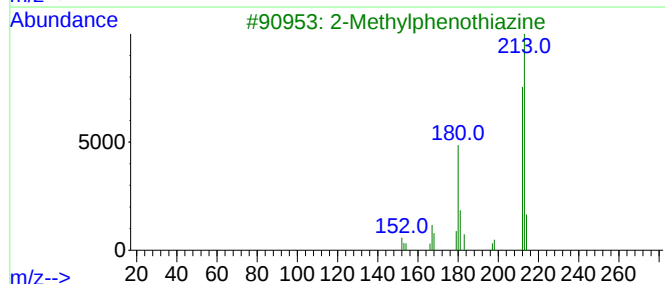
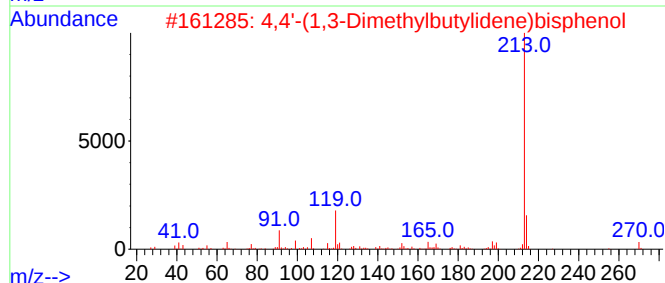
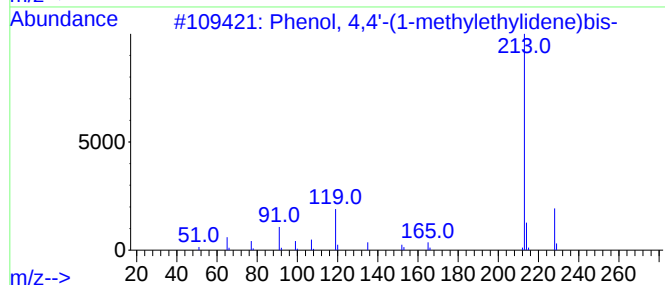
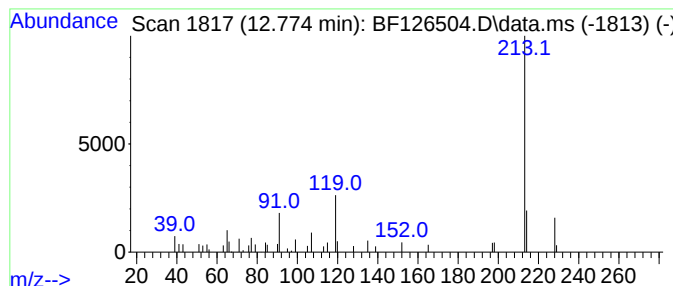
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Peak Number 3 Phenol, 4,4'-(1-methylethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.775	2.13 ng	63824	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	93
2			4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	78
3			2-Methylphenothiazine	213	C13H11NS	005828-51-3	72
4			4-{5H,6H,7H,8H-Imidazo[1,5-a]pyr...	213	C13H15N3	1010409-68-6	59
5			benzenamine, 4-[2-(2-furanyl)eth...	213	C14H15NO	1000400-66-9	53



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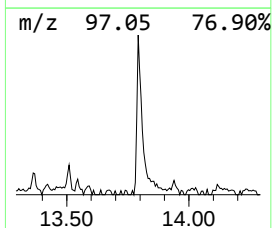
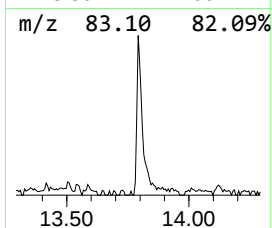
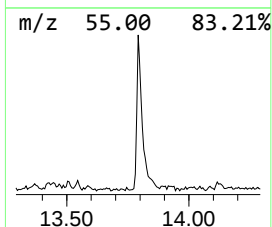
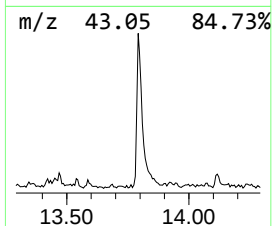
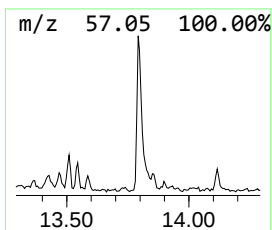
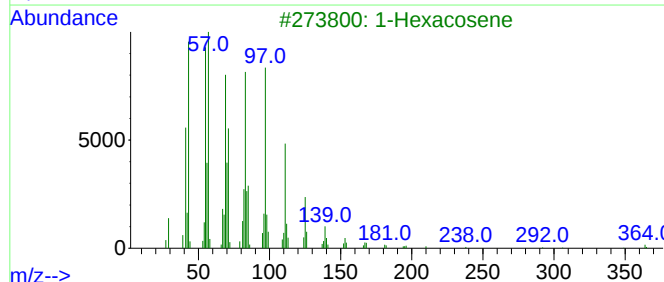
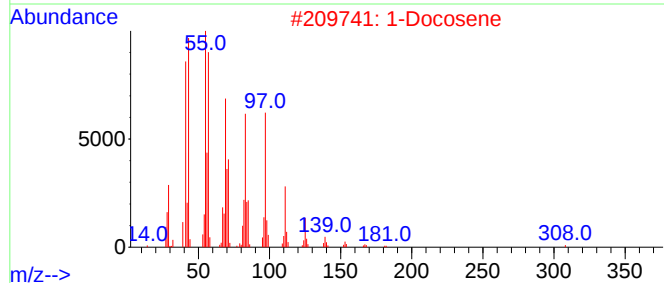
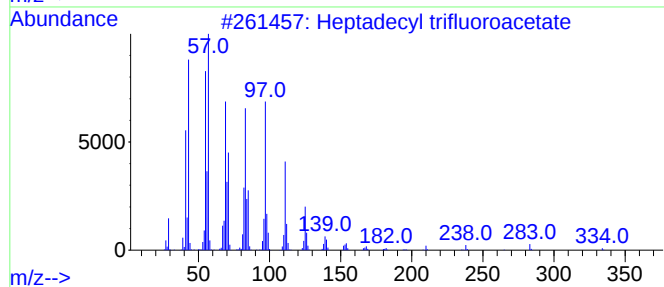
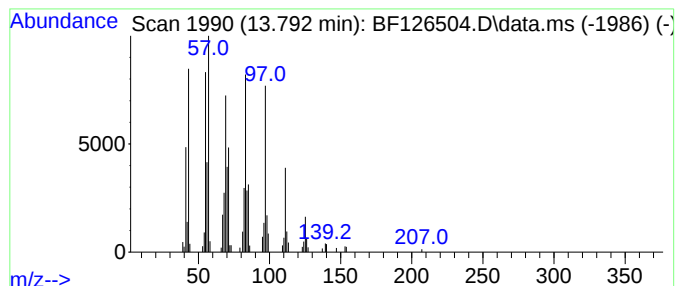
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Peak Number 4 Heptadecyl trifluoroacetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.792	9.59 ng	287423	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
2			1-Docosene	308	C22H44	001599-67-3	91
3			1-Hexacosene	364	C26H52	018835-33-1	91
4			1-Nonadecene	266	C19H38	018435-45-5	91
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



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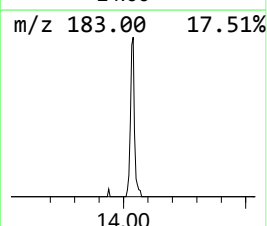
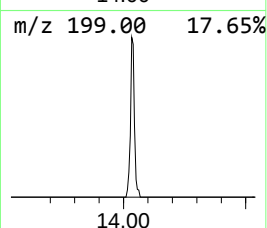
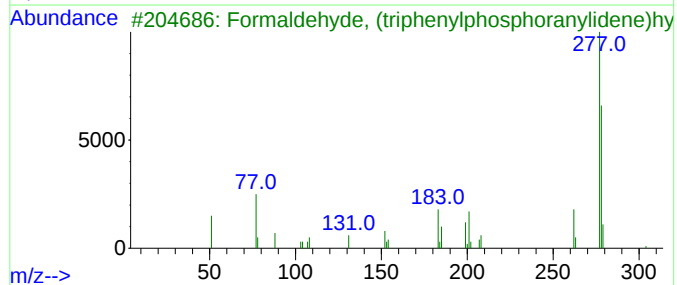
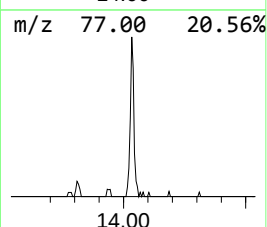
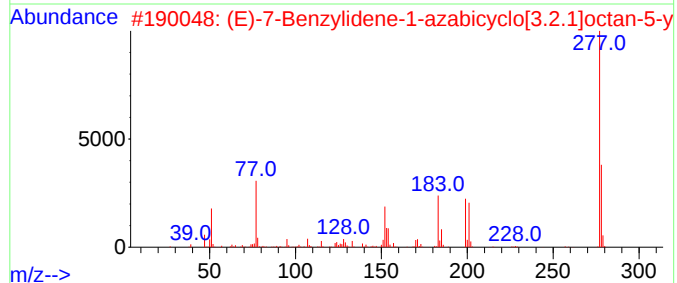
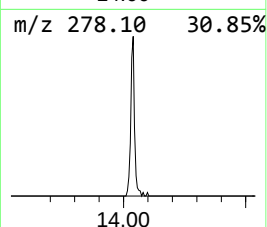
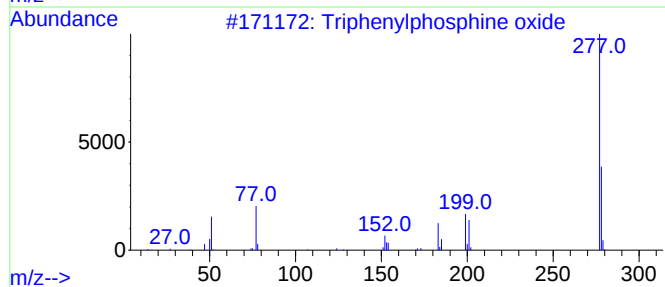
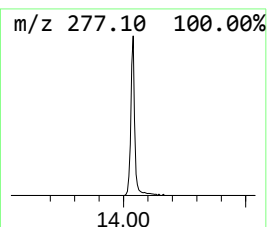
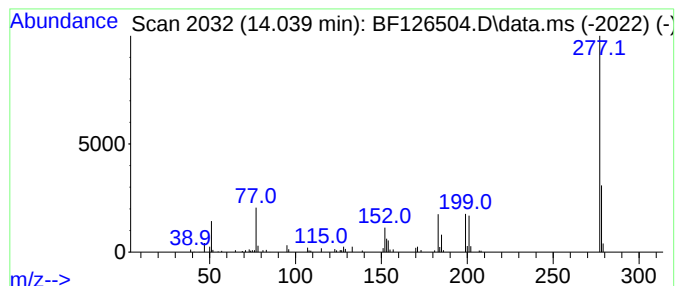
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.039	5.64 ng	169067	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	72
4			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	40
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	37



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COMPOSITE-SAMPLE-1-DEEP

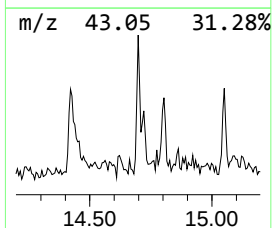
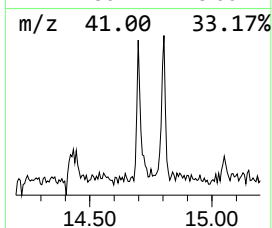
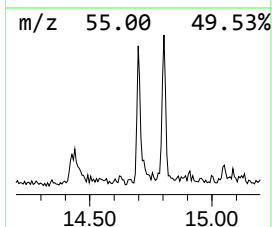
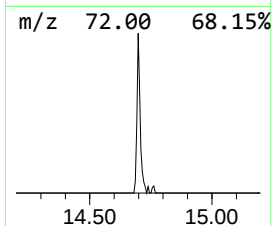
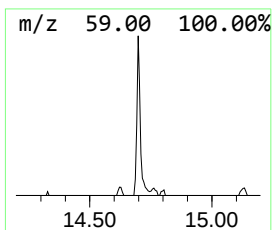
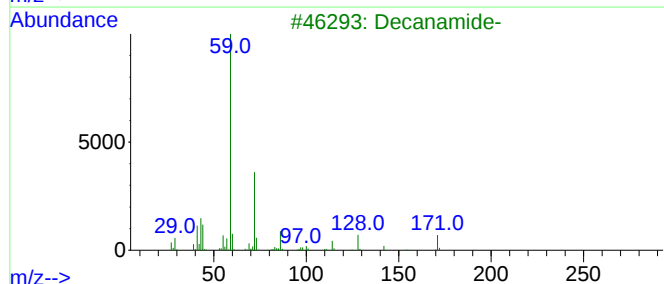
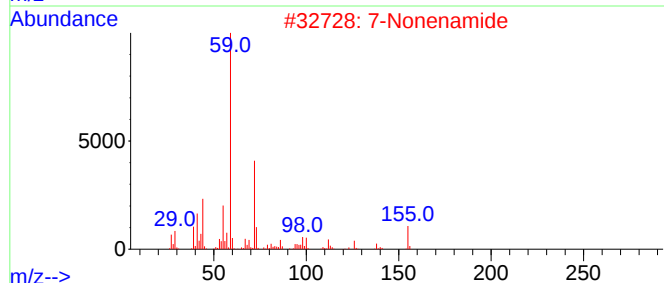
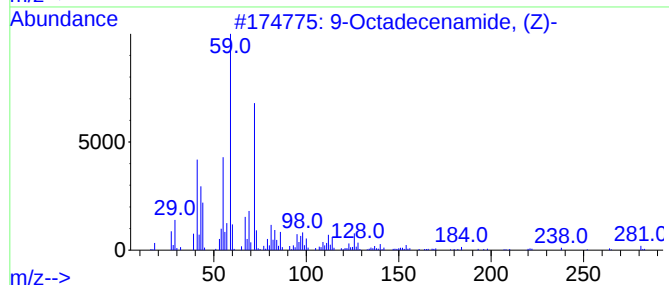
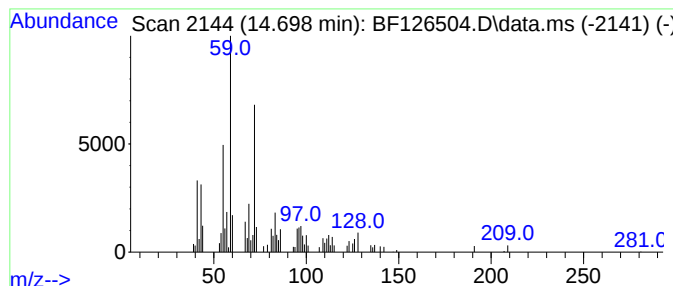
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.698	4.23 ng	102217	Perylene-d12	15.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	78
2			7-Nonenamide	155	C9H17NO	090949-53-4	59
3			Decanamide-	171	C10H21NO	002319-29-1	53
4			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	53
5			Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010522\
Data File : BF126504.D
Acq On : 5 Jan 2022 19:13
Operator : JU/CG
Sample : M5196-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SAMPLE-1-DEEP

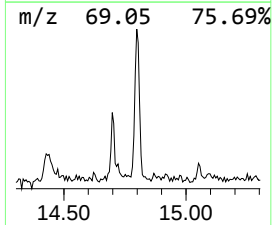
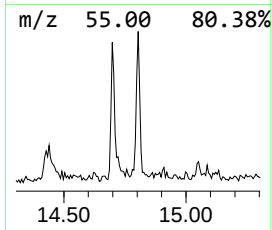
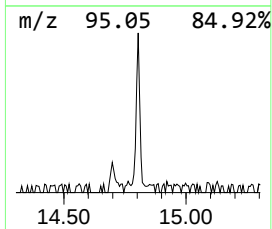
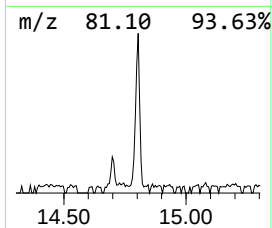
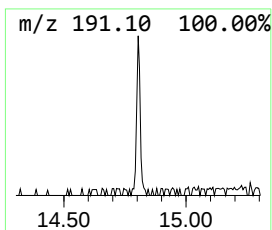
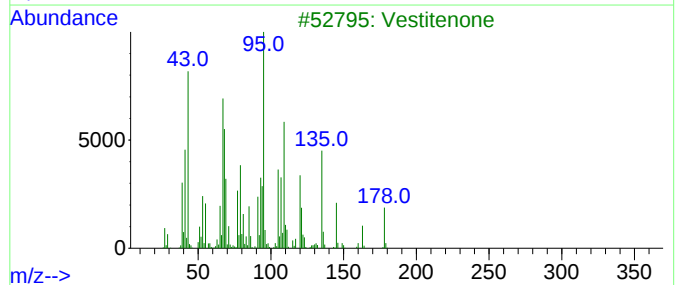
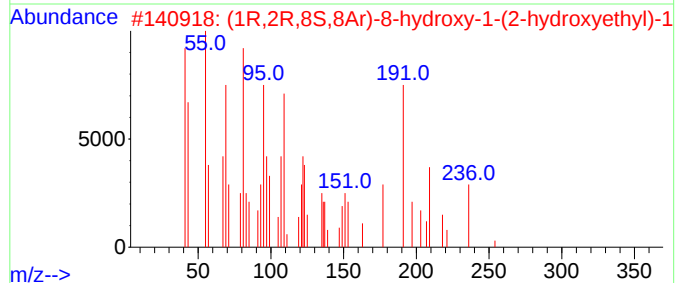
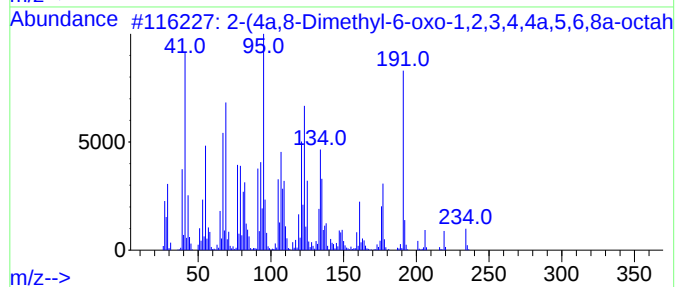
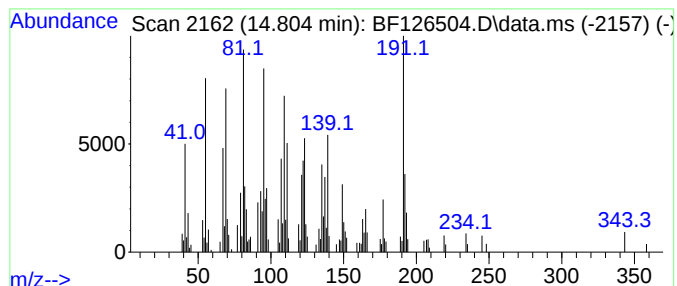
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.804 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	6.93 ng	167440	Perylene-d12	15.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4a,8-Dimethyl-6-oxo-1,2,3,4,4...	234	C15H22O2	1000190-21-8	46		
2	(1R,2R,8S,8Ar)-8-hydroxy-1-(2-hy...	254	C16H30O2	1000298-98-6	43		
3	Vestitenone	178	C12H18O	069401-36-1	38		
4	Amberonne (isomer 2)	234	C16H26O	1010470-69-8	38		
5	Imidazole, 4-methyl-5-[3,3,3-tri...	234	C10H13F3N2O	1000129-15-8	35		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010522\
Data File : BF126504.D
Acq On : 5 Jan 2022 19:13
Operator : JU/CG
Sample : M5196-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SAMPLE-1-DEEP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.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
2-Pentanone, 4-...	4.993	3.0	ng	82860	1	6.781	548131	20.0
n-Hexadecanoic ...	11.839	3.0	ng	114132	4	11.304	758823	20.0
Phenol, 4,4'-(1...	12.775	2.1	ng	63824	5	13.939	599116	20.0
Heptadecyl trif...	13.792	9.6	ng	287423	5	13.939	599116	20.0
Triphenylphosph...	14.039	5.6	ng	169067	5	13.939	599116	20.0
9-Octadecenamid...	14.698	4.2	ng	102217	6	15.380	483120	20.0
unknown14.804	14.804	6.9	ng	167440	6	15.380	483120	20.0