

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
 Data File : BF122191.D
 Acq On : 30 Oct 2020 20:49
 Operator : JU/CG
 Sample : L4541-04
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 124024

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-BF101220.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122191.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.945	483	486	502	rBV	30126	67161	2.54%	0.326%
2	5.339	550	553	578	rBV	1719594	2224934	84.20%	10.795%
3	6.369	725	728	759	rBV	2050832	2477725	93.77%	12.021%
4	6.710	783	786	798	rBV	611851	608175	23.02%	2.951%
5	7.281	880	883	904	rBV	1469432	1564546	59.21%	7.591%
6	7.992	1001	1004	1023	rBV	796882	834804	31.59%	4.050%
7	9.069	1183	1187	1197	rBV	2707224	2642329	100.00%	12.820%
8	9.186	1203	1207	1213	rVB	49818	48473	1.83%	0.235%
9	9.469	1252	1255	1269	rVB	541091	502086	19.00%	2.436%
10	9.745	1298	1302	1313	rBV	1052231	959801	36.32%	4.657%
11	10.539	1433	1437	1452	rBV	1715316	1734881	65.66%	8.417%
12	11.233	1552	1555	1566	rBV	1045621	1064182	40.27%	5.163%
13	11.763	1643	1645	1651	rVB3	58071	72248	2.73%	0.351%
14	12.292	1732	1735	1737	rBV	34871	42057	1.59%	0.204%
15	12.457	1760	1763	1769	rBV	143012	164726	6.23%	0.799%
16	12.686	1799	1802	1808	rVB	145546	172028	6.51%	0.835%
17	12.815	1820	1824	1829	rBV	2858745	2471996	93.55%	11.994%
18	13.710	1973	1976	1983	rBV	287637	408152	15.45%	1.980%
19	13.880	2001	2005	2010	rBV	692900	742937	28.12%	3.605%
20	14.327	2078	2081	2083	rBV3	48017	48385	1.83%	0.235%
21	14.357	2083	2086	2093	rVB5	53155	96257	3.64%	0.467%
22	14.762	2152	2155	2159	rVB	100086	94405	3.57%	0.458%
23	14.939	2179	2185	2189	rBV2	121208	206942	7.83%	1.004%
24	14.980	2189	2192	2199	rVV5	60633	114055	4.32%	0.553%
25	15.209	2229	2231	2238	rVB	36196	51641	1.95%	0.251%
26	15.274	2239	2242	2246	rVV2	49993	77608	2.94%	0.377%
27	15.315	2246	2249	2260	rVB	398714	579853	21.94%	2.813%
28	15.486	2275	2278	2283	rBV3	39921	48427	1.83%	0.235%
29	15.698	2310	2314	2319	rVB	122416	166239	6.29%	0.807%
30	15.774	2322	2327	2338	rVB6	46774	129935	4.92%	0.630%
31	17.203	2564	2570	2583	rBV4	66899	193956	7.34%	0.941%

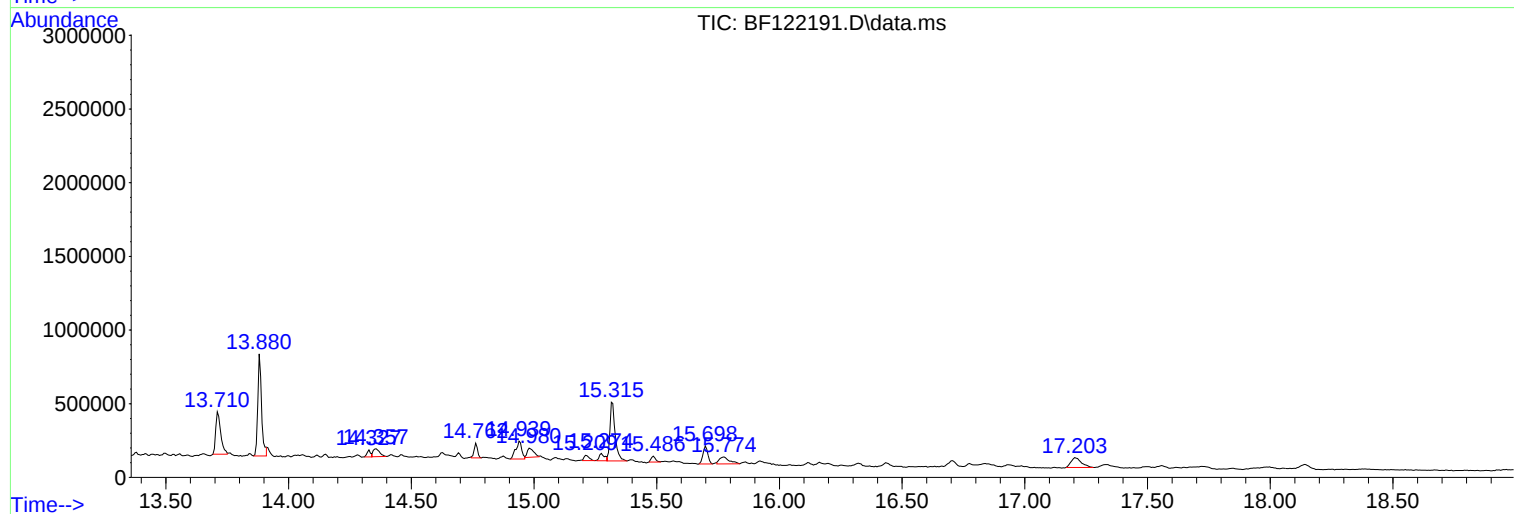
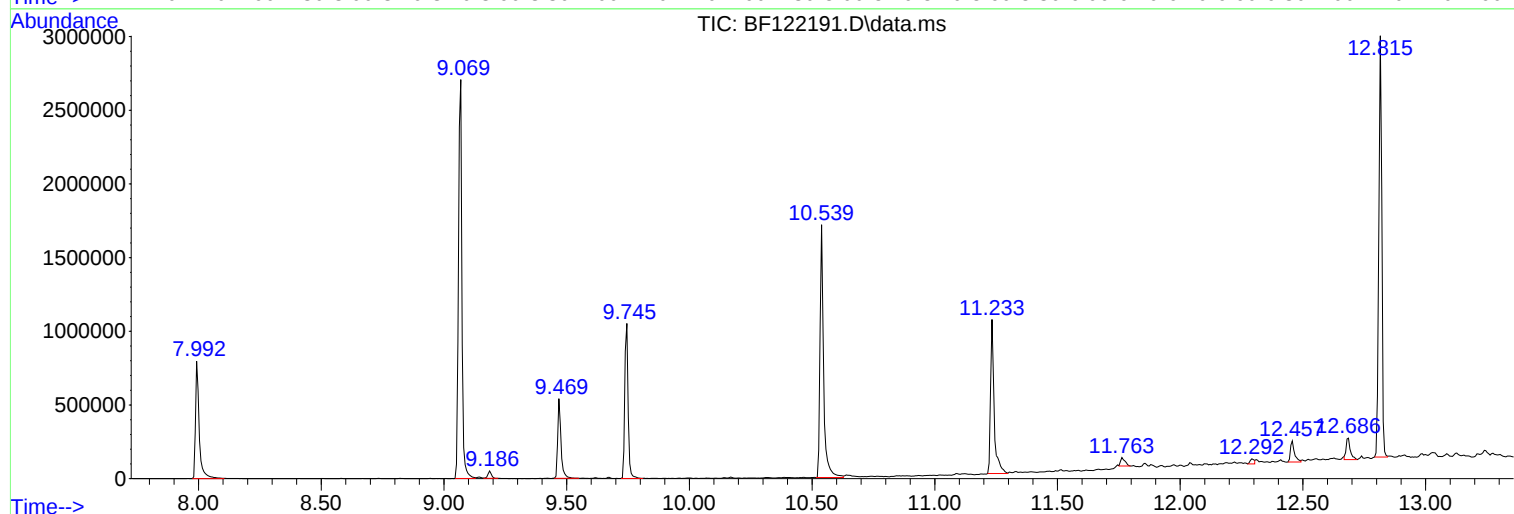
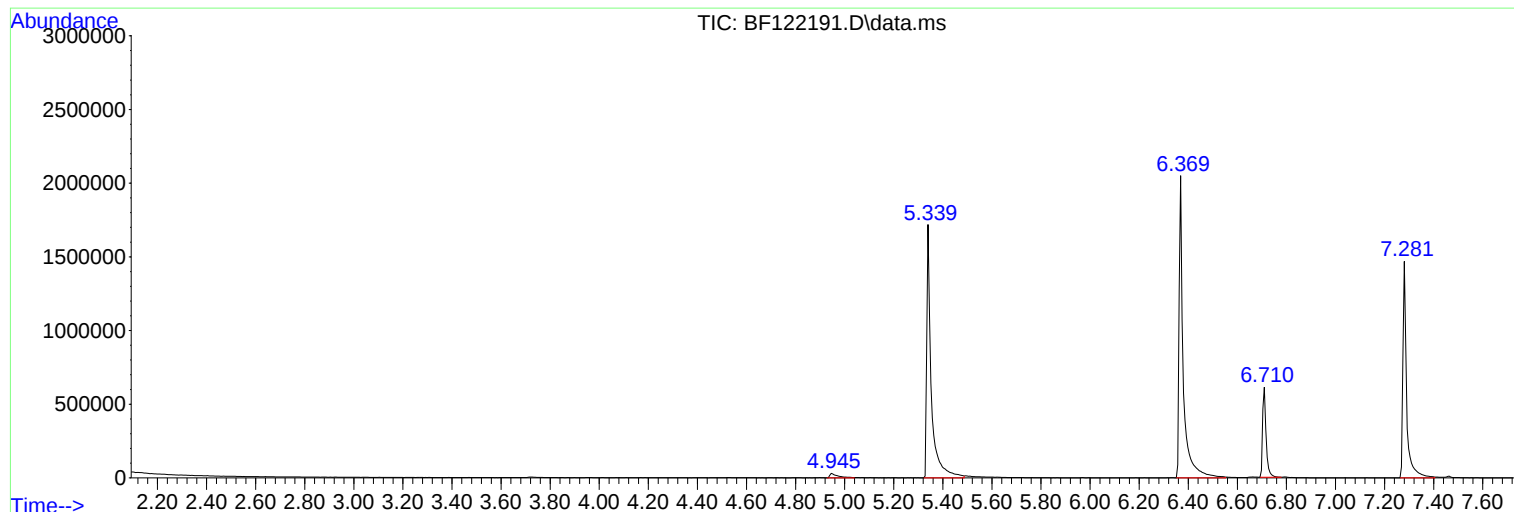
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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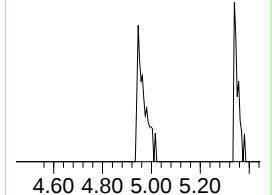
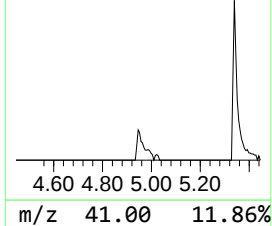
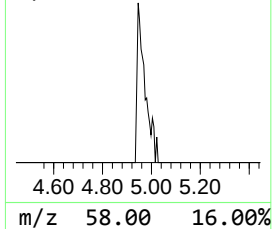
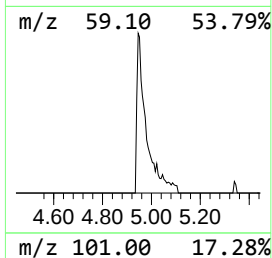
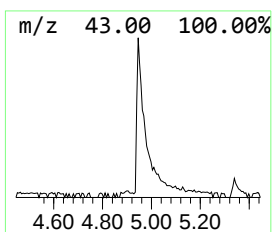
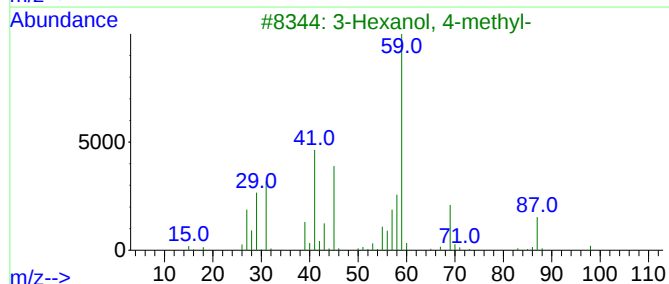
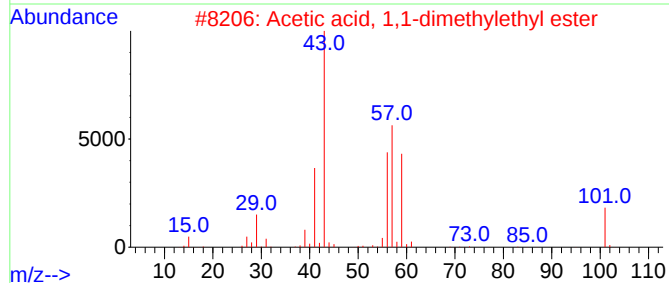
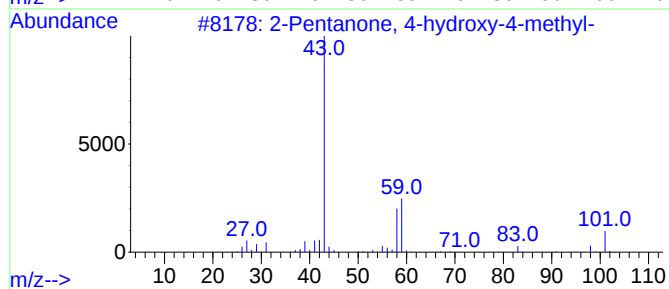
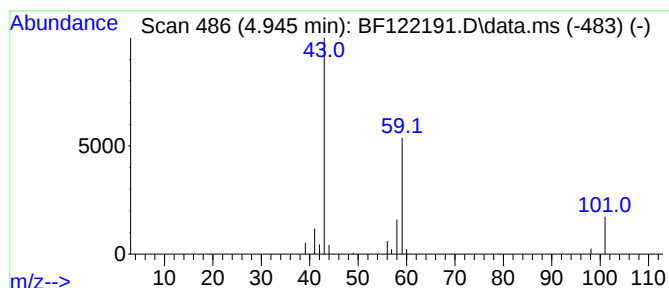
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TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.945	2.21 ng	67161	1,4-Dichlorobenzene-d4	6.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9		
4	3-Hexanol	102	C6H14O	000623-37-0	9		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9		



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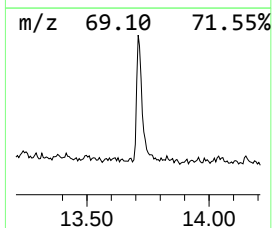
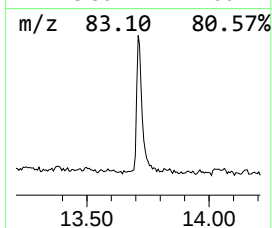
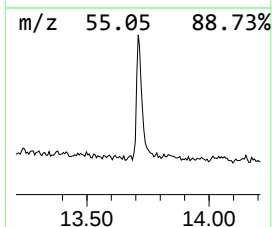
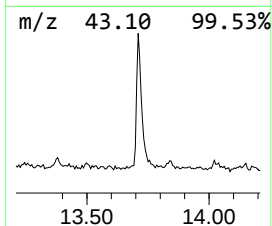
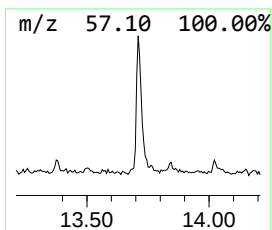
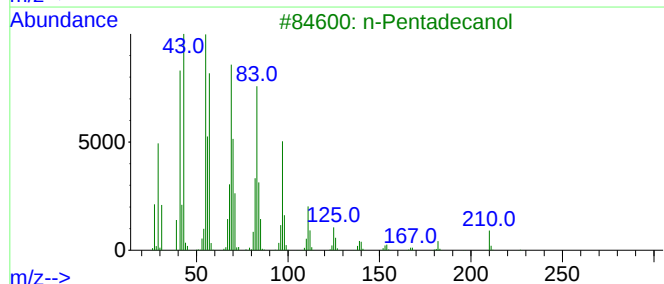
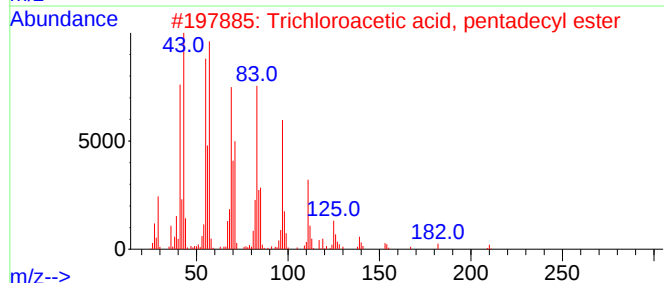
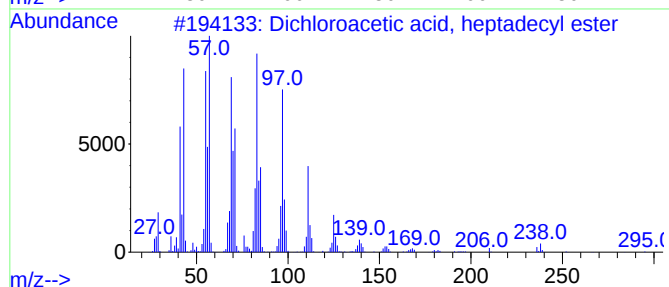
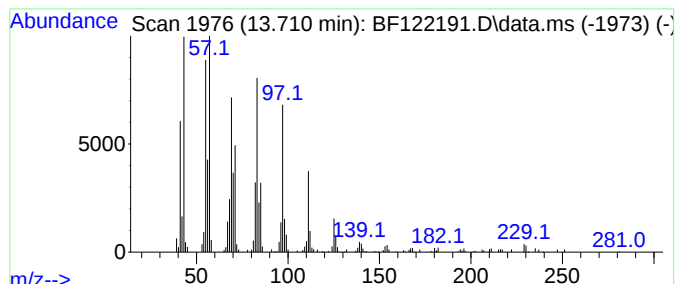
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Peak Number 2 Dichloroacetic acid, heptad... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.710	10.99 ng	408152	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3			n-Pentadecanol	228	C15H32O	000629-76-5	93
4			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
5			Behenic alcohol	326	C22H46O	000661-19-8	91



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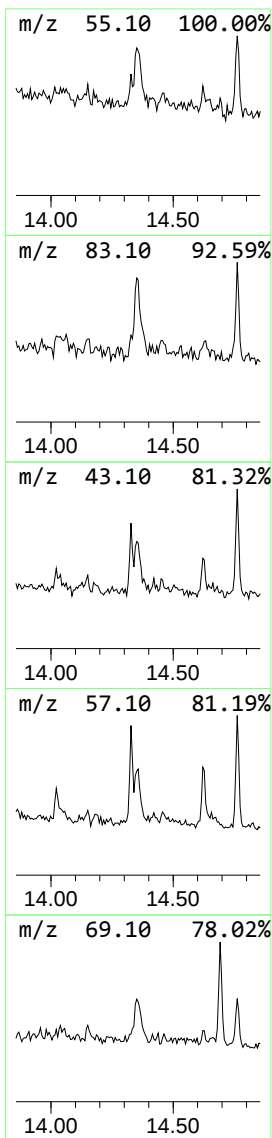
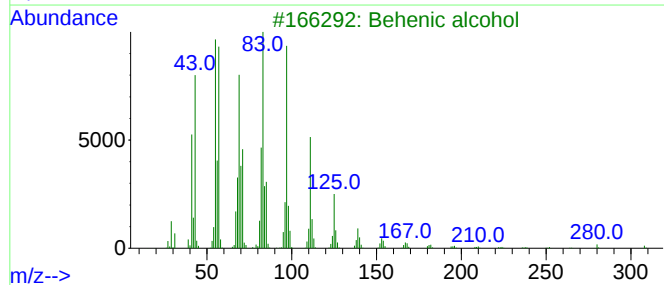
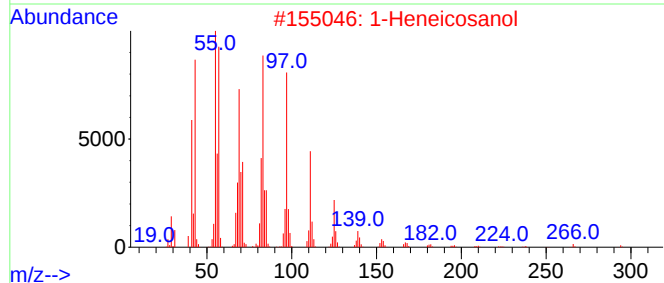
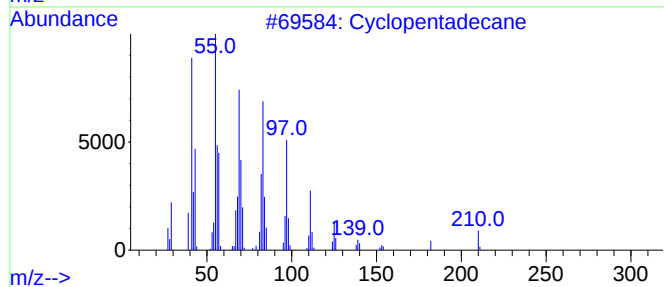
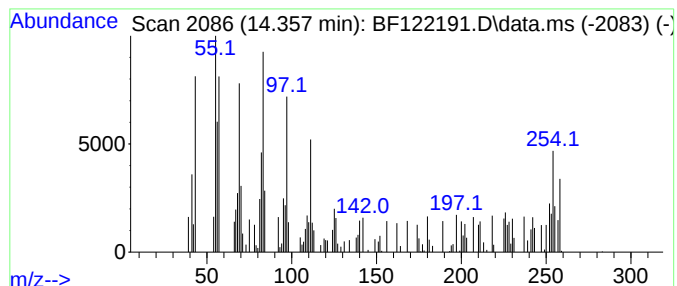
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Peak Number 3 Cyclopentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.357	2.59 ng	96257	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	78
2			1-Heneicosanol	312	C21H44O	015594-90-8	64
3			Behenic alcohol	326	C22H46O	000661-19-8	64
4			1-Heptacosanol	396	C27H56O	002004-39-9	64
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	64



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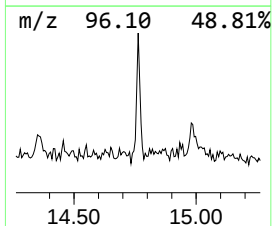
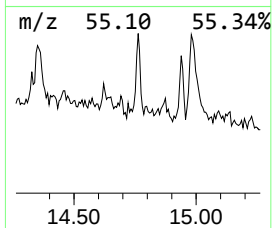
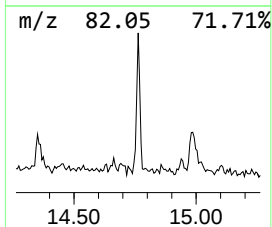
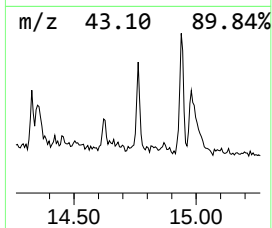
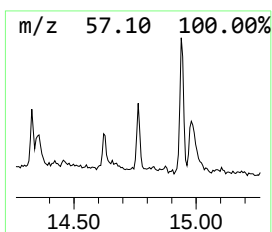
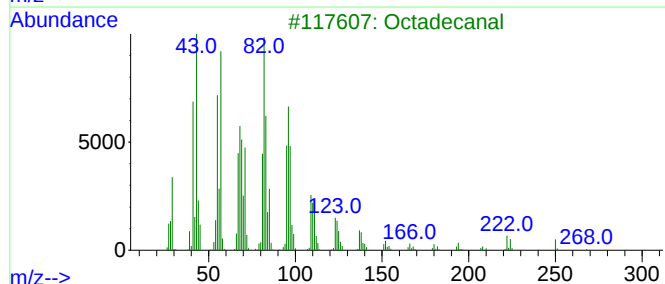
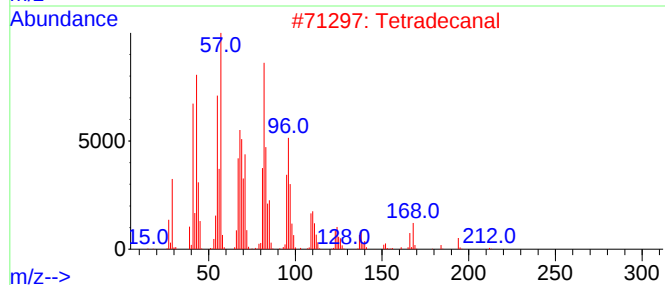
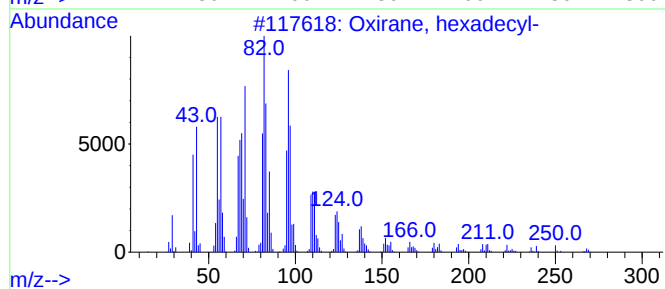
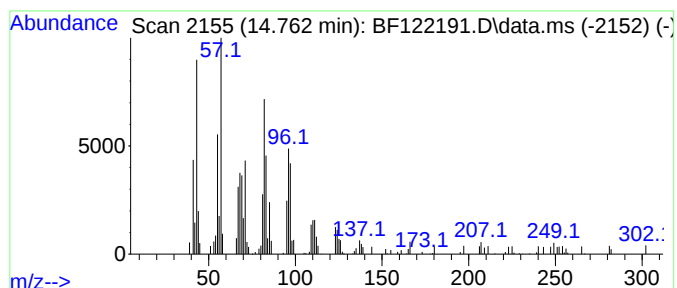
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Peak Number 4 Oxirane, hexadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.762	3.26 ng	94405	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2			Tetradecanal	212	C14H28O	000124-25-4	74
3			Octadecanal	268	C18H36O	000638-66-4	68
4			Hexadecanal	240	C16H32O	000629-80-1	68
5			13-Octadecenal	266	C18H34O	056554-90-6	64



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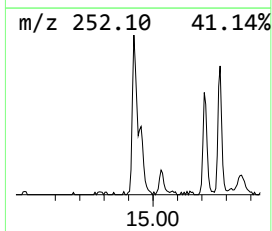
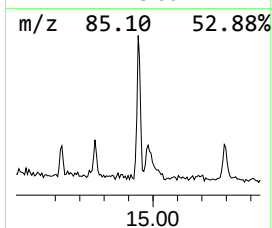
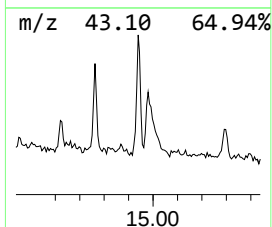
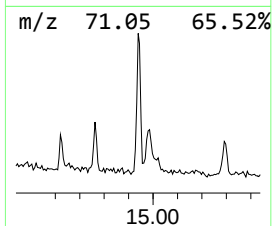
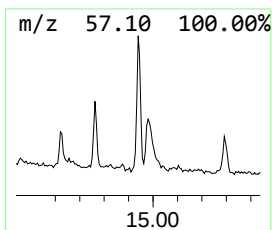
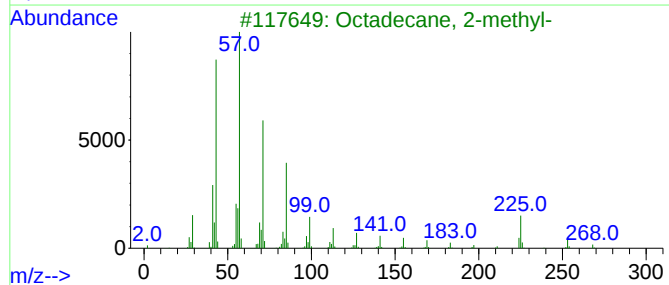
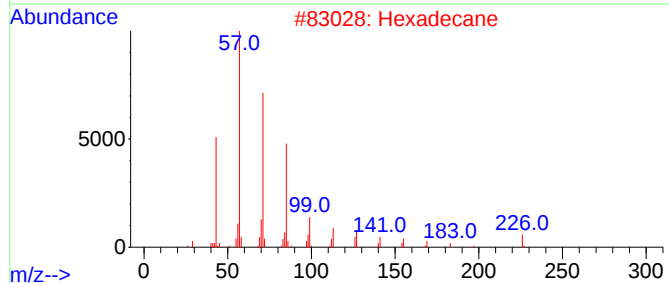
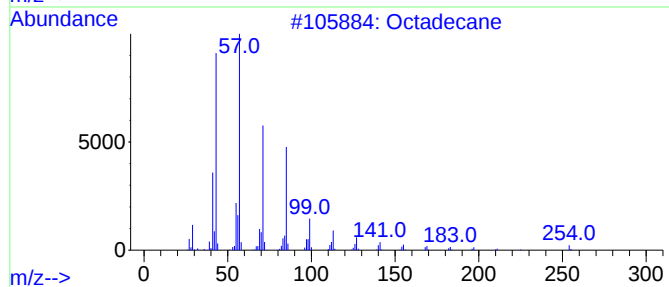
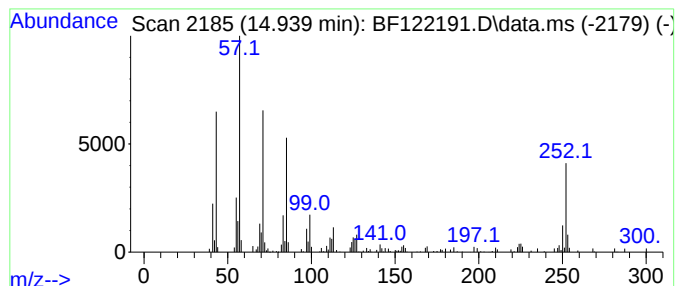
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Peak Number 5 Octadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	7.14 ng	206942	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	87
2			Hexadecane	226	C16H34	000544-76-3	87
3			Octadecane, 2-methyl-	268	C19H40	001560-88-9	70
4			Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	64
5			Heneicosane	296	C21H44	000629-94-7	62



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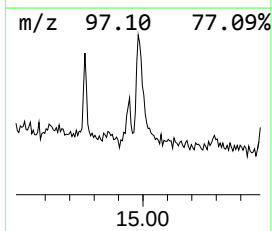
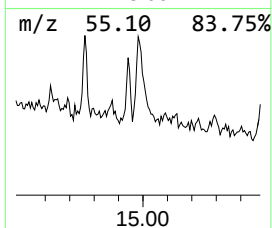
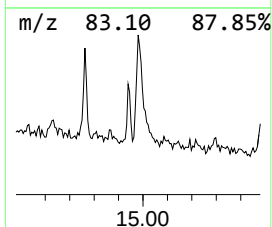
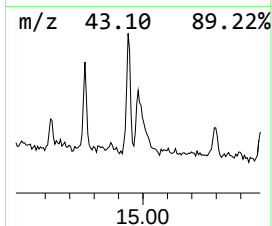
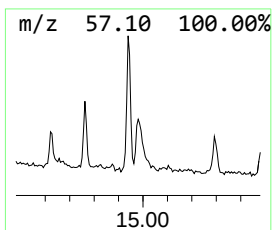
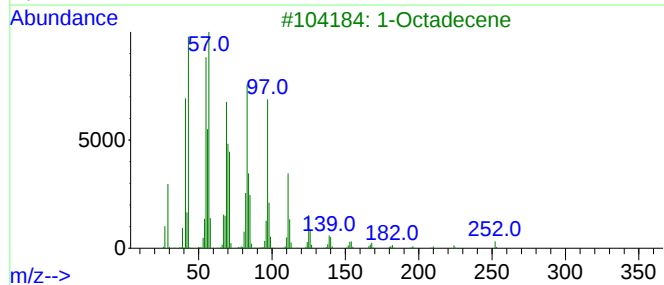
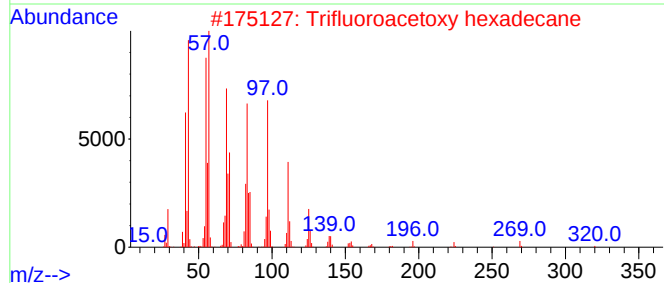
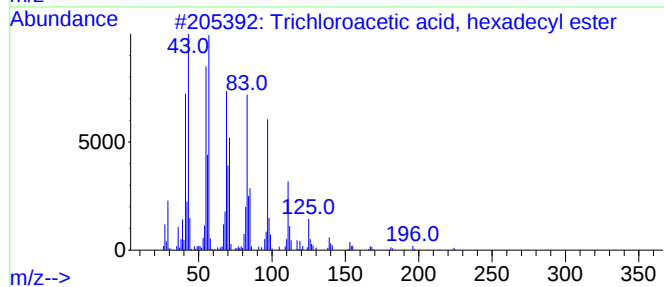
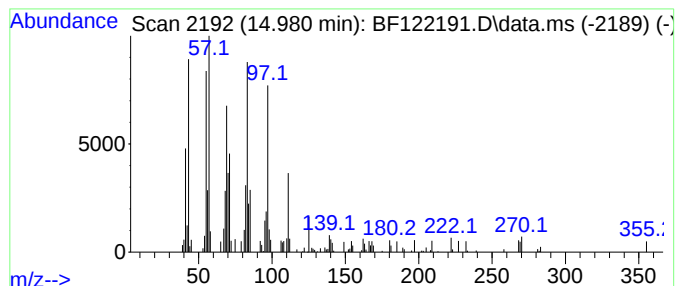
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.980	3.93 ng	114055	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	86
3			1-Octadecene	252	C18H36	000112-88-9	80
4			1-Heptacosanol	396	C27H56O	002004-39-9	76
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122191.D
Acq On : 30 Oct 2020 20:49
Operator : JU/CG
Sample : L4541-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
124024

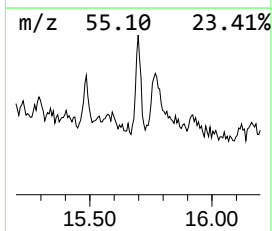
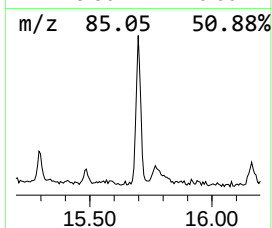
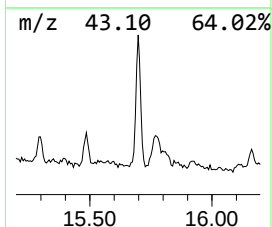
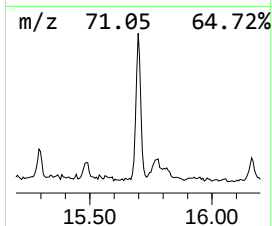
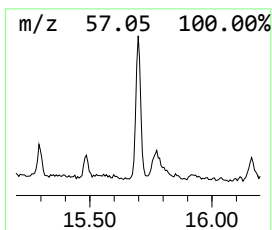
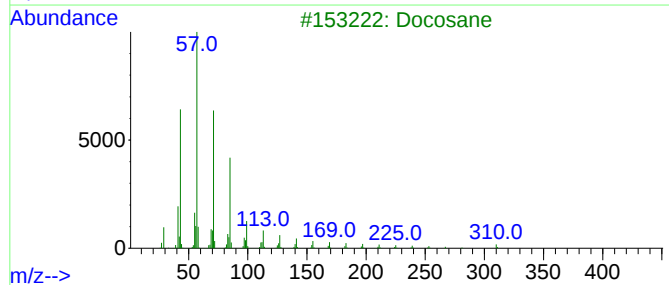
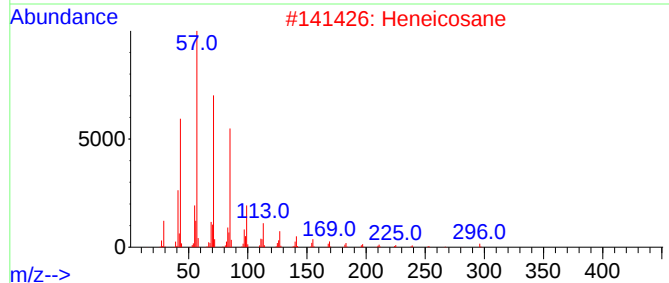
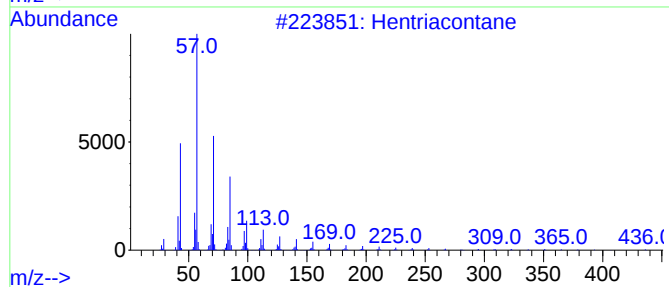
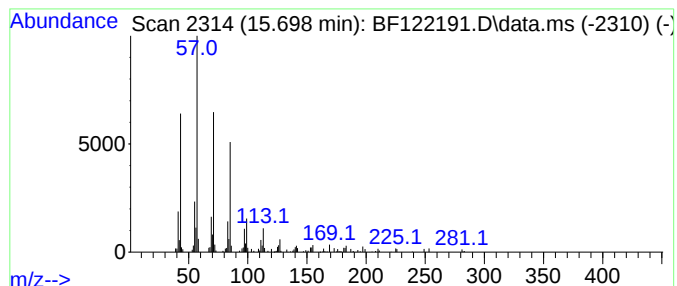
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hentriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.698	5.73 ng	166239	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Heneicosane	296	C21H44	000629-94-7	87
3			Docosane	310	C22H46	000629-97-0	86
4			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
5			2-Bromotetradecane	276	C14H29Br	074036-95-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122191.D
Acq On : 30 Oct 2020 20:49
Operator : JU/CG
Sample : L4541-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

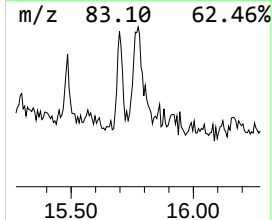
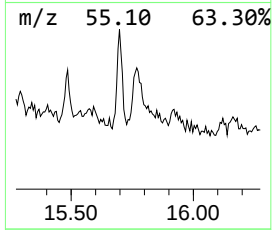
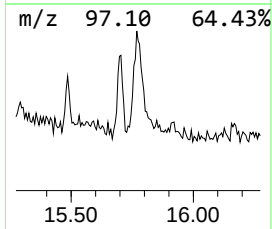
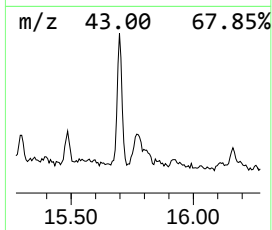
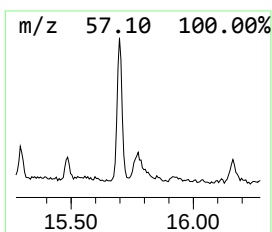
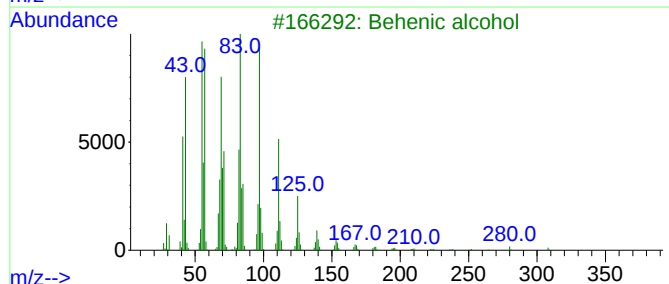
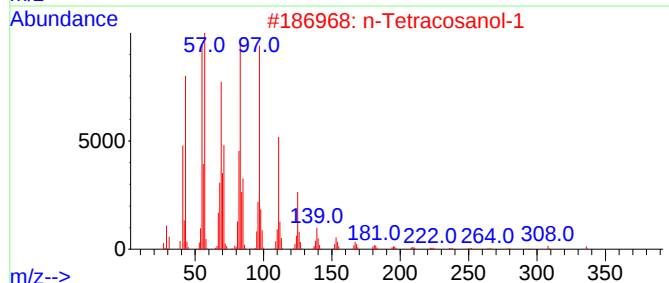
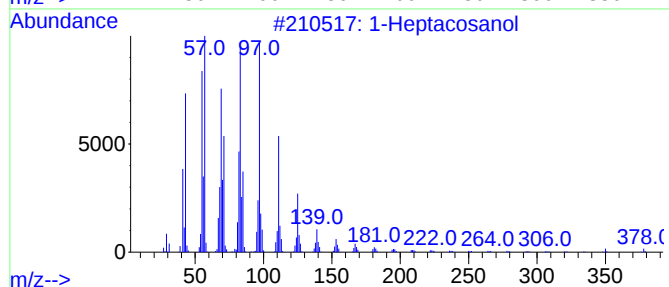
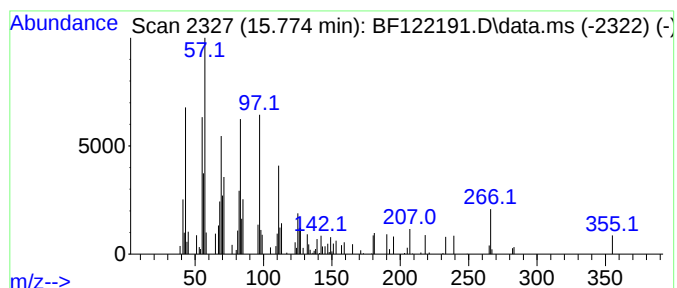
Instrument :
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ClientSampled :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.774	4.48 ng	129935	Perylene-d12	15.315	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	Behenic alcohol	326	C22H46O	000661-19-8	92
4	4-Methyl-E-9-octadecene	266	C19H38	1000130-87-1	81
5	Z-5-Nonadecene	266	C19H38	1000131-11-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122191.D
Acq On : 30 Oct 2020 20:49
Operator : JU/CG
Sample : L4541-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
124024

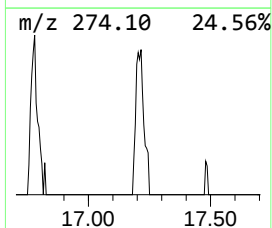
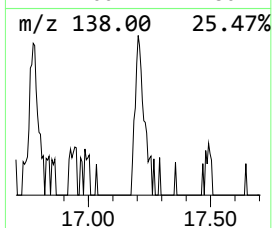
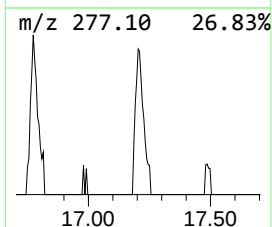
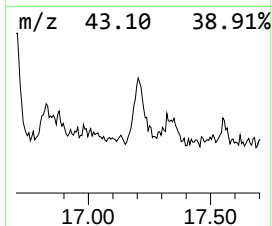
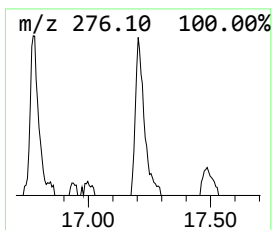
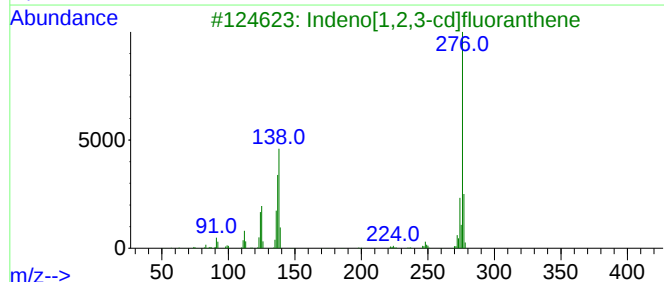
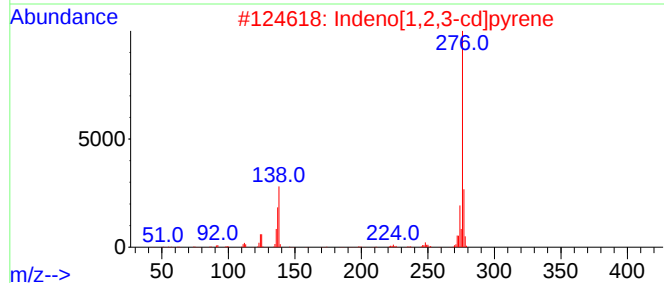
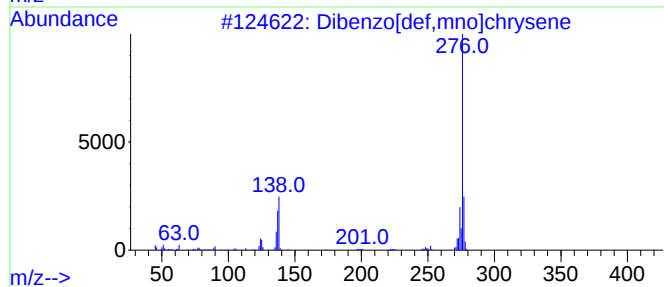
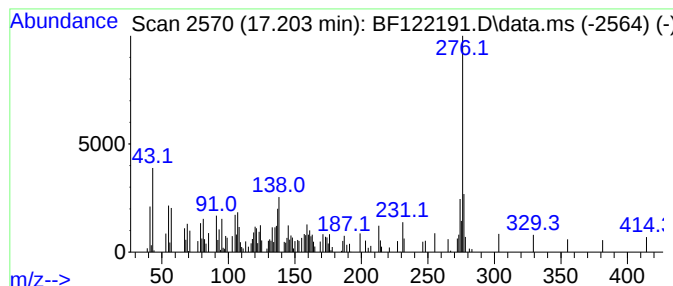
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Dibenzo[def,mno]chrysene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.203	6.69 ng	193956	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	93
2			Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	76
3			Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	76
4			Benzo[ghi]perylene	276	C22H12	000191-24-2	76
5			7H-Furo[3,2-g][1]benzopyran-7-on...	276	C14H12O6	018646-72-5	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122191.D
Acq On : 30 Oct 2020 20:49
Operator : JU/CG
Sample : L4541-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.945	2.2	ng	67161	1	6.710	608175	20.0
Dichloroacetic ...	13.710	11.0	ng	408152	5	13.880	742937	20.0
Cyclopentadecane	14.357	2.6	ng	96257	5	13.880	742937	20.0
Oxirane, hexade...	14.762	3.3	ng	94405	6	15.315	579853	20.0
Octadecane	14.939	7.1	ng	206942	6	15.315	579853	20.0
Trichloroacetic...	14.980	3.9	ng	114055	6	15.315	579853	20.0
Hentriacontane	15.698	5.7	ng	166239	6	15.315	579853	20.0
1-Heptacosanol	15.774	4.5	ng	129935	6	15.315	579853	20.0
Dibenzo[def,mno...	17.203	6.7	ng	193956	6	15.315	579853	20.0