

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122922\
 Data File : BF131878.D
 Acq On : 29 Dec 2022 15:15
 Operator : CG\JU
 Sample : N6231-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3S

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-BF122422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131878.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.034	495	501	513	rVB	693044	1013345	33.96%	5.035%
2	5.440	565	570	573	rBV	2474817	2374469	79.57%	11.798%
3	6.457	737	743	746	rBV	2096227	2486975	83.34%	12.357%
4	6.816	800	804	807	rBV	602900	494355	16.57%	2.456%
5	7.387	895	901	904	rBV	1534934	1623410	54.40%	8.066%
6	8.104	1018	1023	1027	rBV	726896	646324	21.66%	3.211%
7	9.186	1201	1207	1210	rBV	3141733	2984227	100.00%	14.828%
8	9.869	1313	1323	1326	rBV	892231	787641	26.39%	3.914%
9	10.586	1440	1445	1449	rBV	169763	136399	4.57%	0.678%
10	10.663	1452	1458	1461	rBV	2356597	2086917	69.93%	10.369%
11	11.357	1572	1576	1579	rBV	878495	805392	26.99%	4.002%
12	11.380	1579	1580	1584	rVB	58957	38441	1.29%	0.191%
13	11.892	1663	1667	1671	rBV	187812	160627	5.38%	0.798%
14	12.574	1776	1783	1787	rBV	76503	70929	2.38%	0.352%
15	12.804	1818	1822	1827	rVB	66716	79025	2.65%	0.393%
16	12.957	1843	1848	1851	rBV	3008642	2601859	87.19%	12.928%
17	13.521	1939	1944	1947	rBV2	36532	36630	1.23%	0.182%
18	13.845	1996	1999	2011	rBV	246284	320826	10.75%	1.594%
19	14.010	2022	2027	2030	rBV	589877	530944	17.79%	2.638%
20	14.110	2037	2044	2048	rBV	200278	234368	7.85%	1.165%
21	14.480	2103	2107	2113	rBV4	26155	49144	1.65%	0.244%
22	15.057	2202	2205	2212	rVB	27727	45328	1.52%	0.225%
23	15.421	2264	2267	2272	rVB	26886	34161	1.14%	0.170%
24	15.486	2274	2278	2287	rVB	326393	431855	14.47%	2.146%
25	16.009	2362	2367	2376	rBV9	23076	52200	1.75%	0.259%

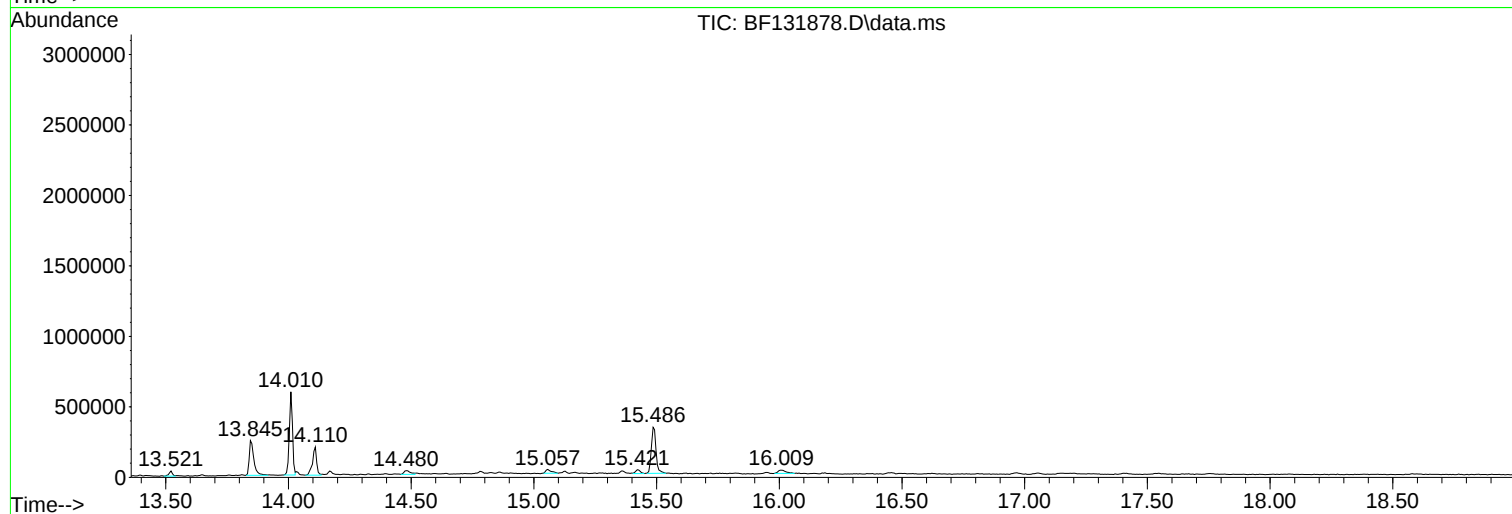
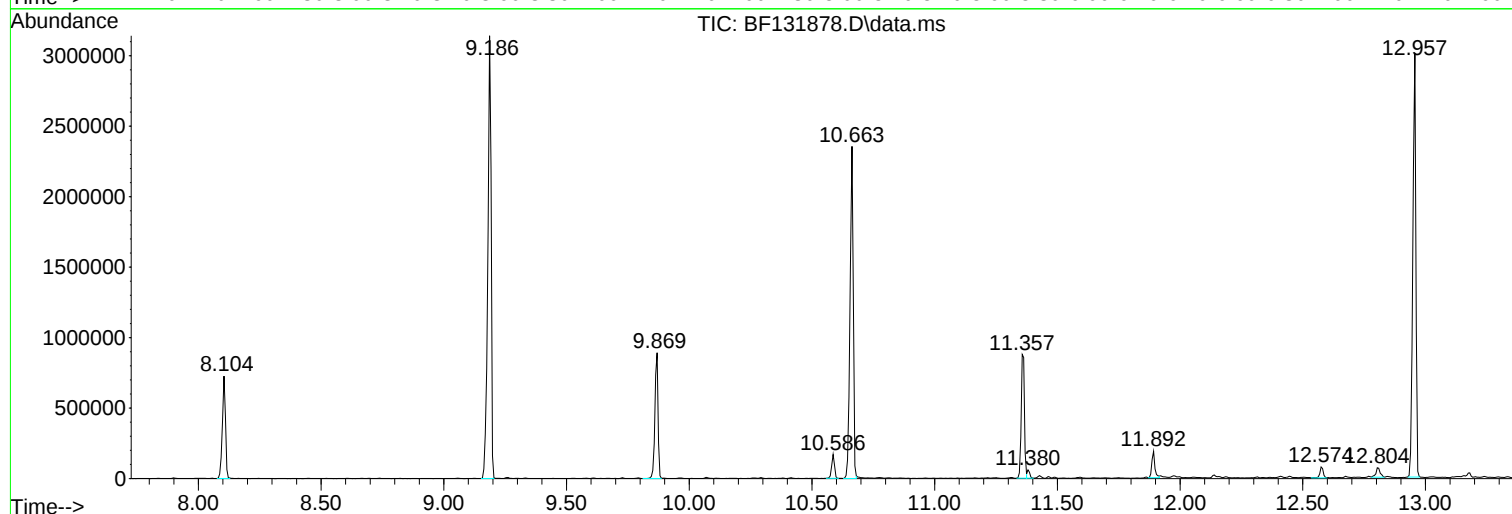
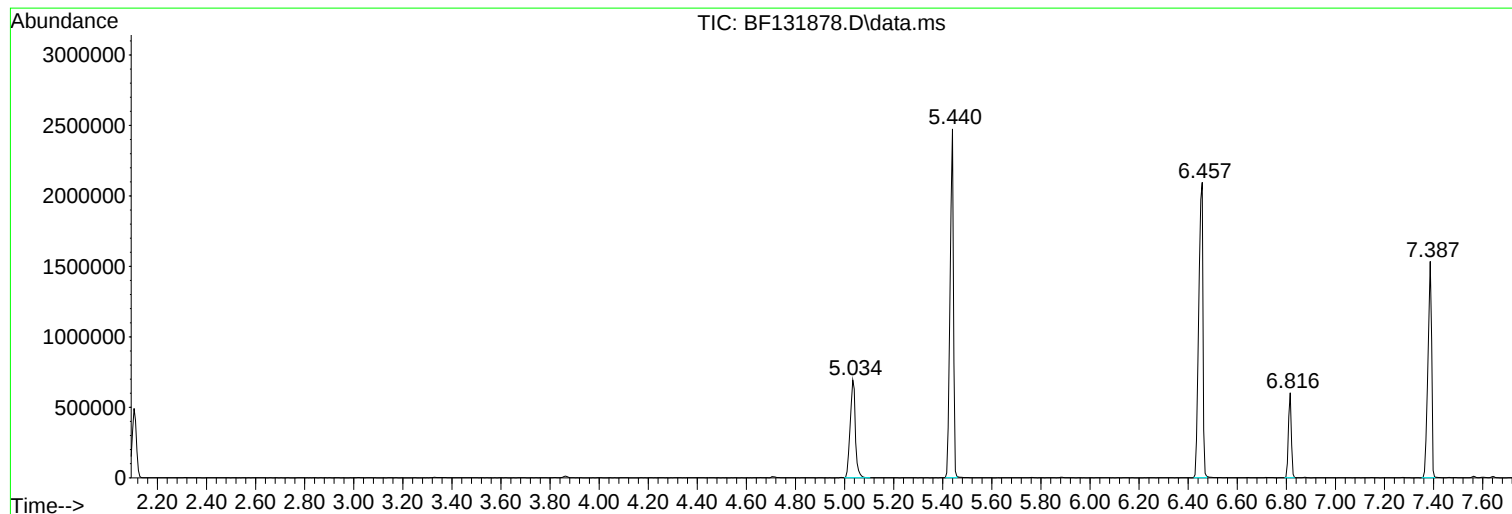
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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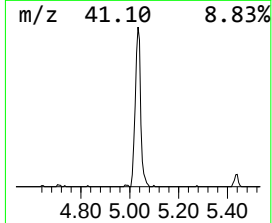
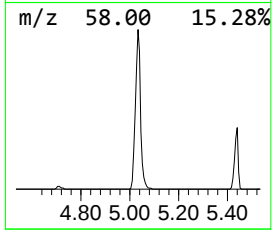
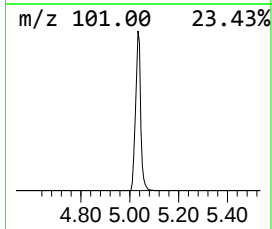
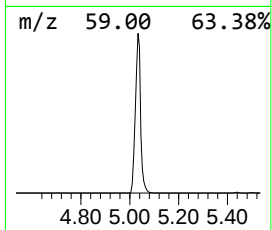
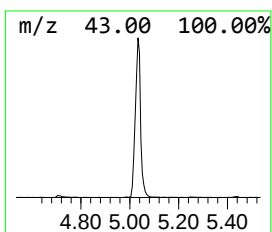
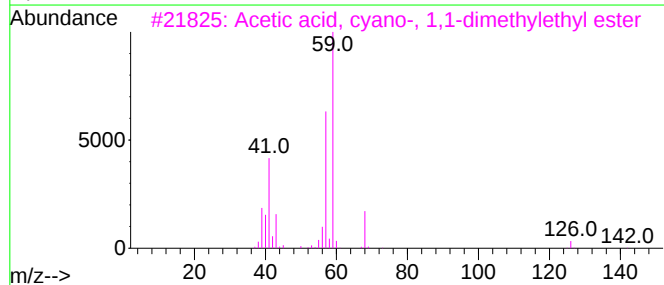
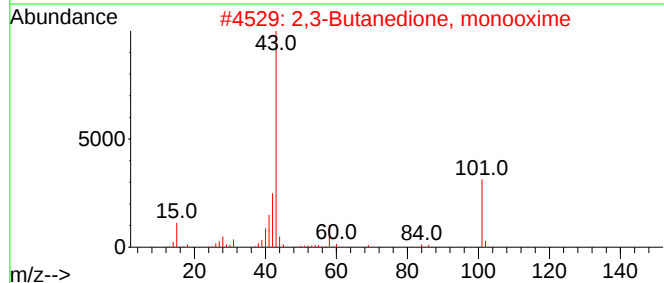
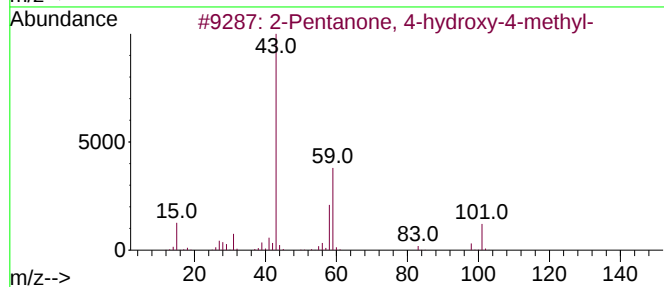
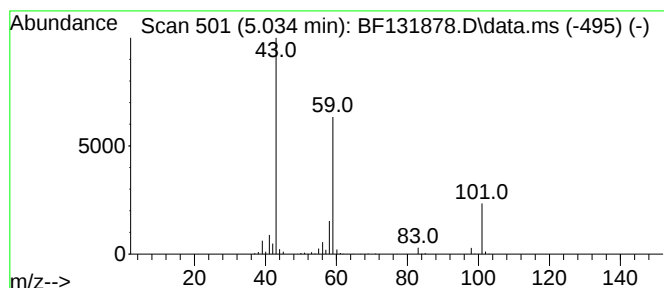
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.034	41.00 ng	1013350	1,4-Dichlorobenzene-d4	6.816	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
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	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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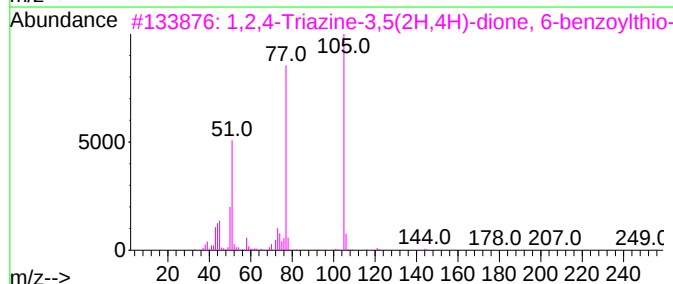
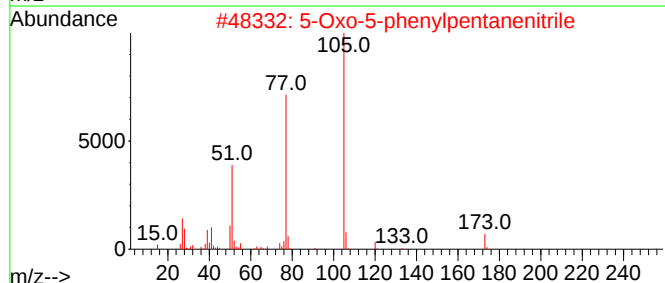
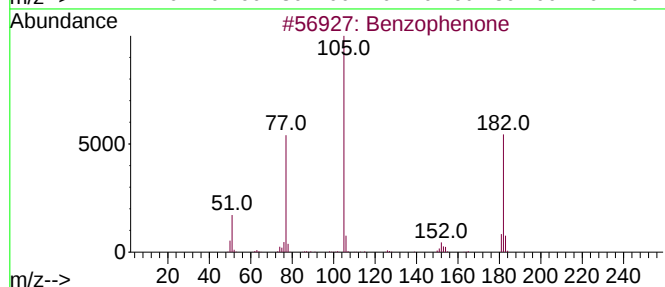
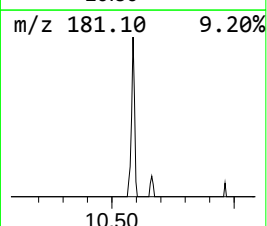
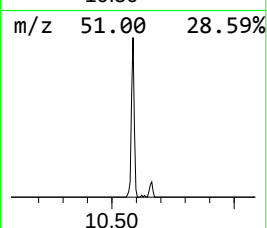
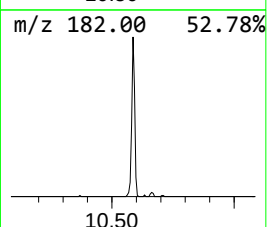
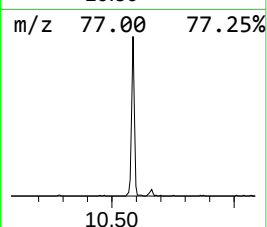
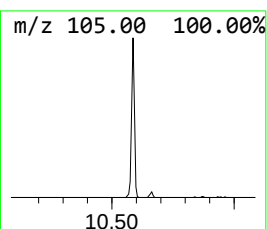
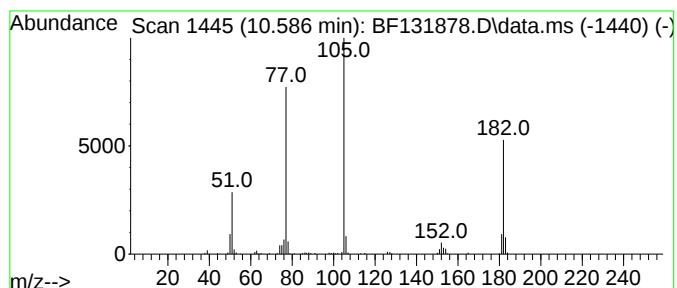
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	3.46 ng	136399	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	53
3			1,2,4-Triazine-3,5(2H,4H)-dione,...	249	C10H7N3O3S	024168-34-1	53
4			Benzoic acid, 3,5-difluophenyl e...	234	C13H8F2O2	1000357-79-5	53
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	53



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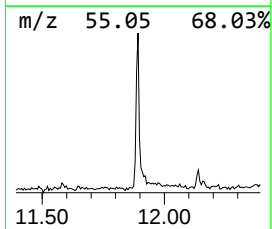
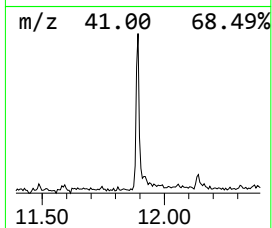
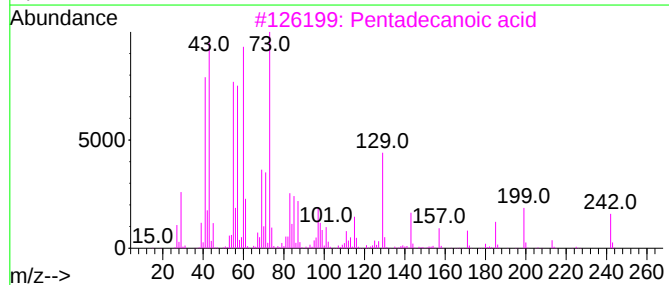
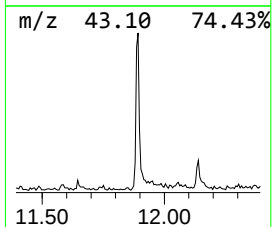
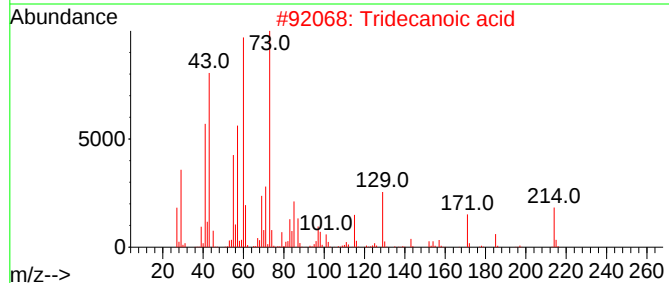
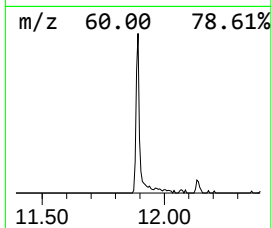
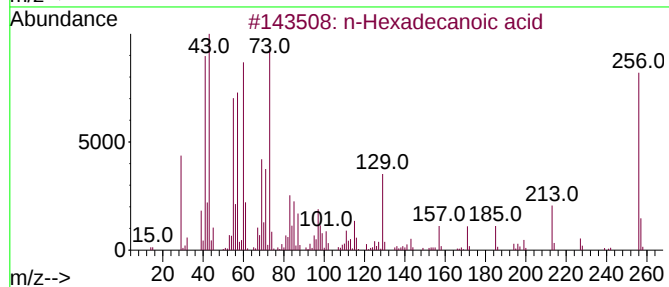
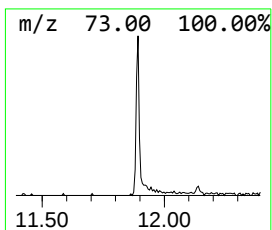
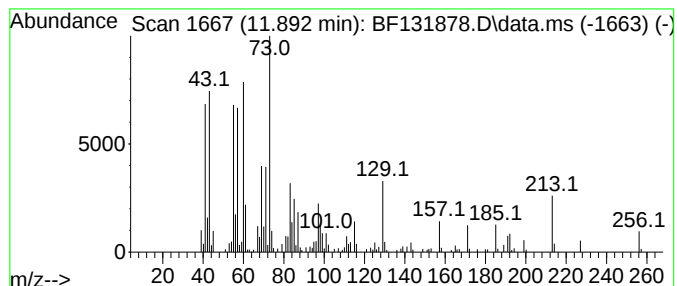
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.892	3.99 ng	160627	Phenanthrene-d10		11.363	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	70
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	68
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	64
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	55



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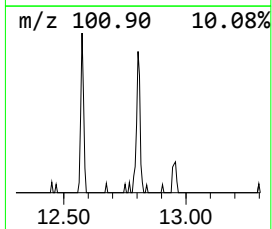
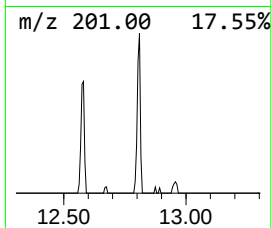
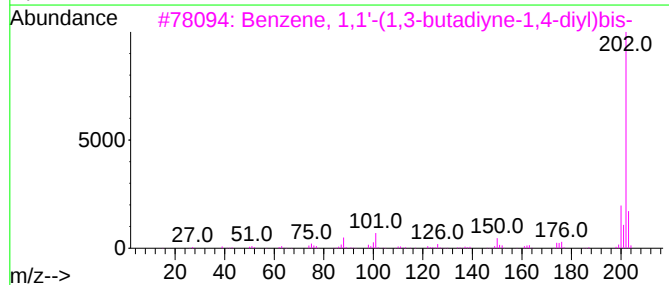
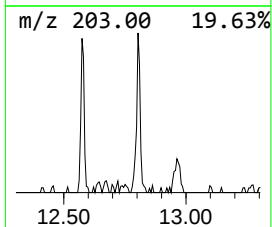
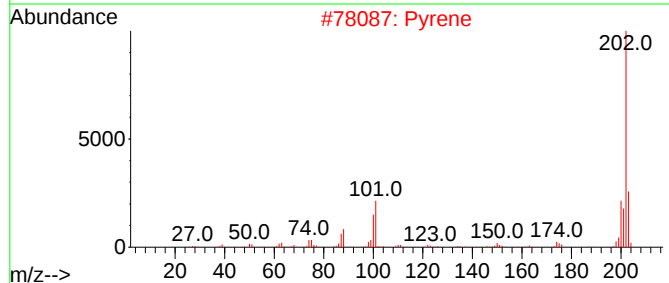
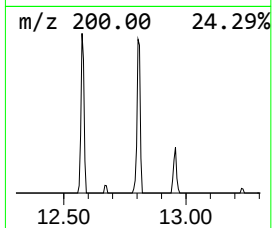
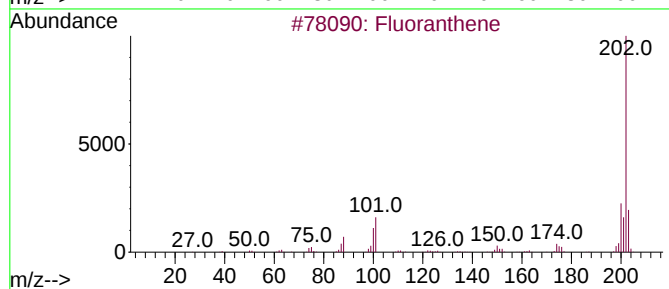
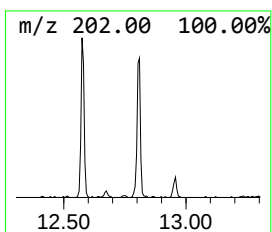
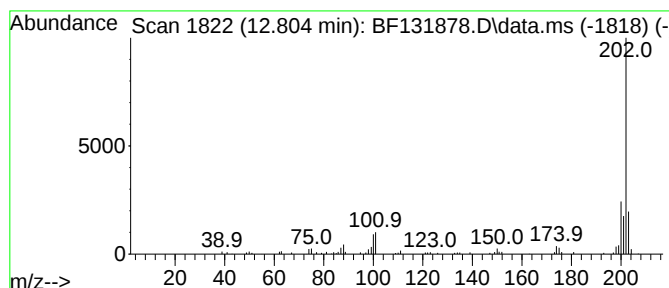
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Peak Number 4 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.804	2.98 ng	79025	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fluoranthene	202	C16H10	000206-44-0	95
2			Pyrene	202	C16H10	000129-00-0	93
3			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	72
4			4-Bromobenzoic acid, undecyl ester	354	C18H27BrO2	1000282-84-5	12
5			Benzaldehyde, 2,6-difuloro-3,4-d...	202	C9H8F2O3	152434-99-6	9



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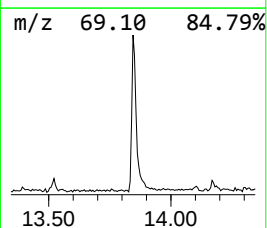
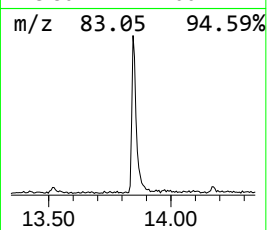
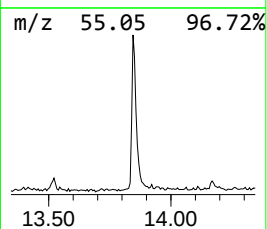
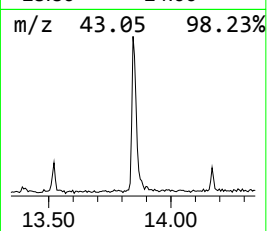
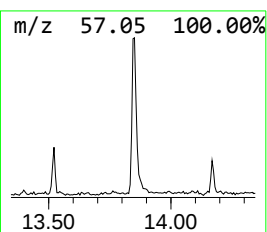
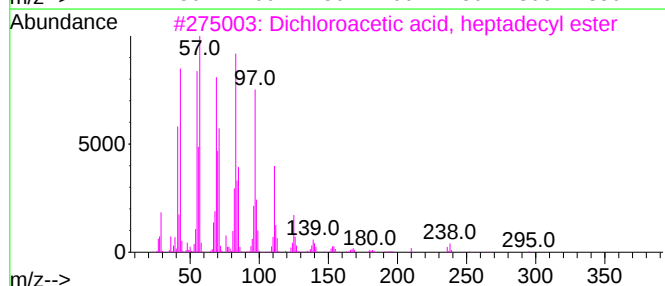
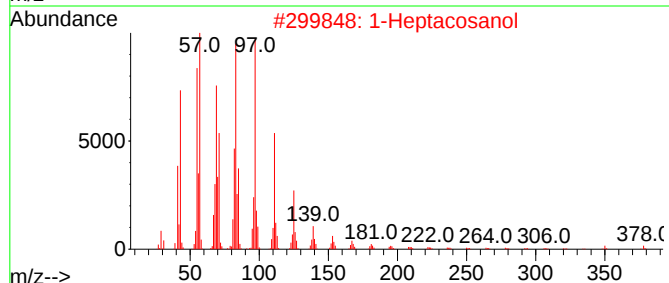
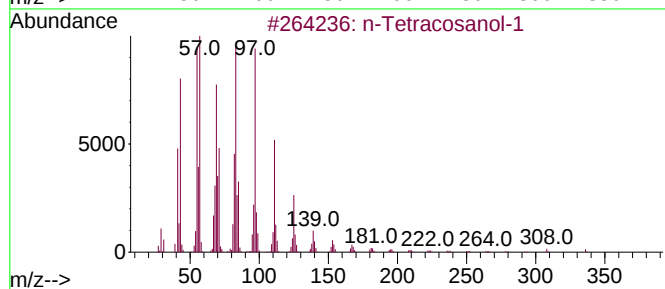
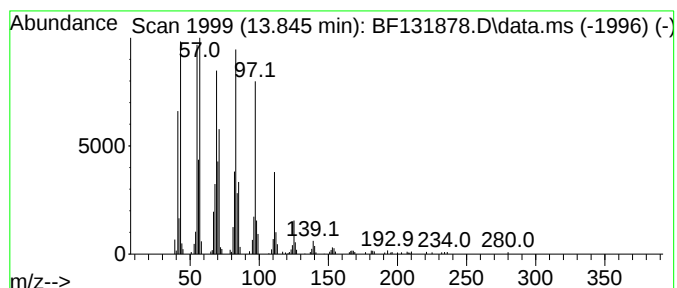
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Peak Number 5 n-Tetracosanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	12.09 ng	320826	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2			1-Heptacosanol	396	C27H56O	002004-39-9	94
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4			Behenic alcohol	326	C22H46O	000661-19-8	94
5			1-Hexacosene	364	C26H52	018835-33-1	94



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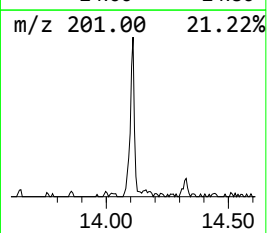
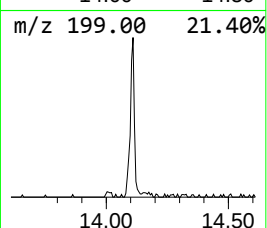
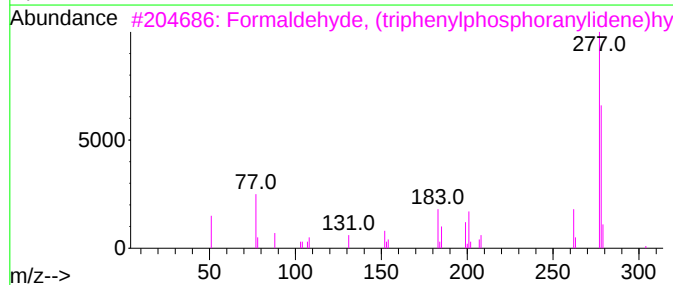
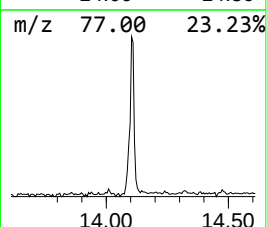
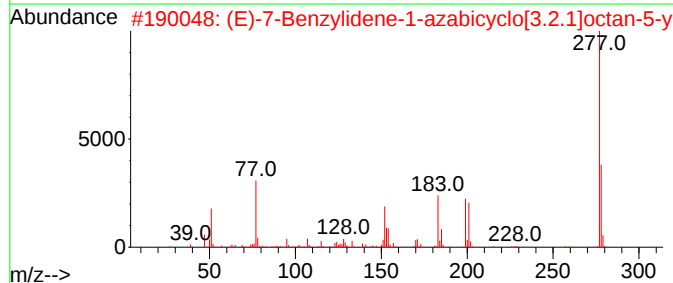
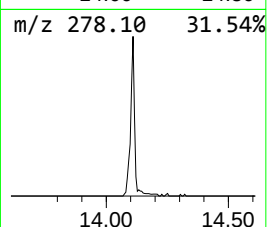
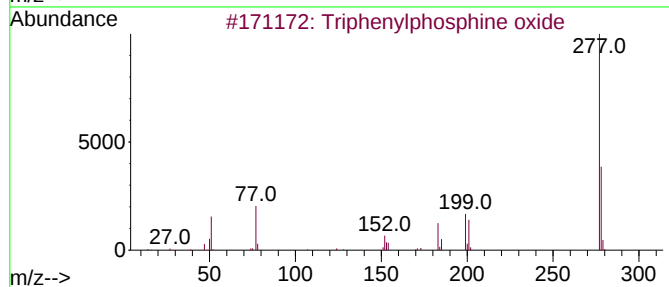
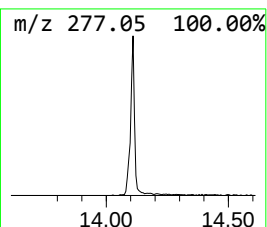
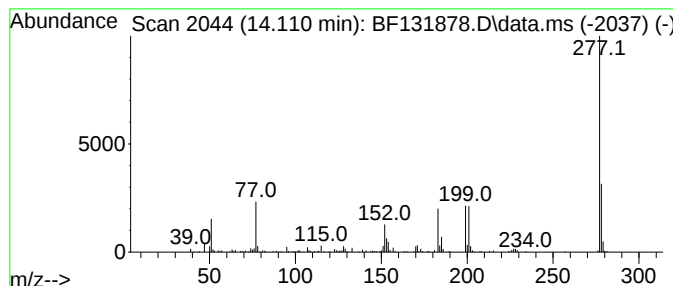
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.110	8.83 ng	234368	Chrysene-d12	14.010

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	52
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	32
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122922\
Data File : BF131878.D
Acq On : 29 Dec 2022 15:15
Operator : CG\JU
Sample : N6231-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3S

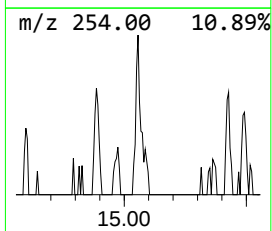
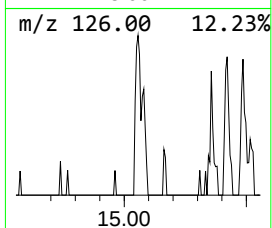
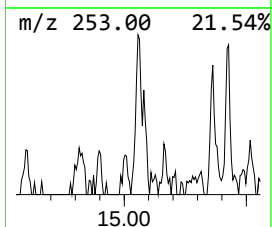
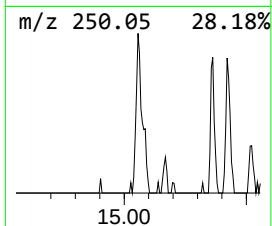
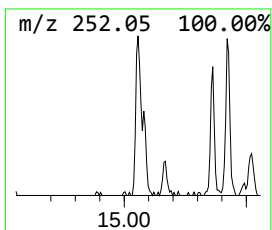
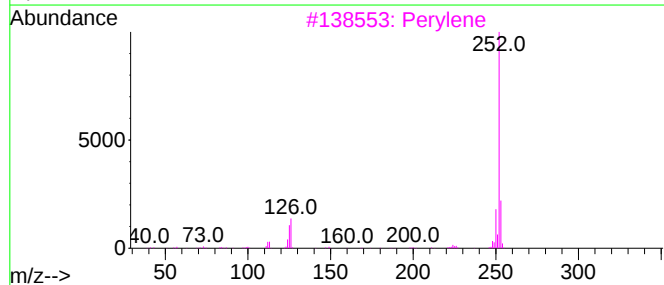
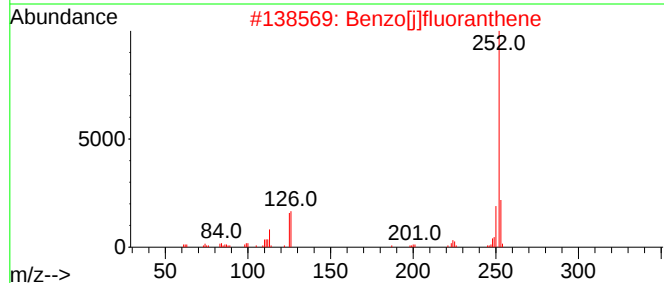
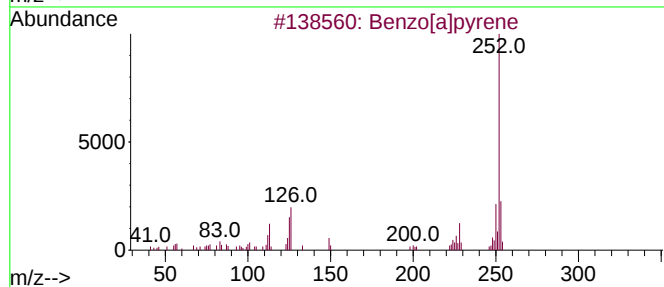
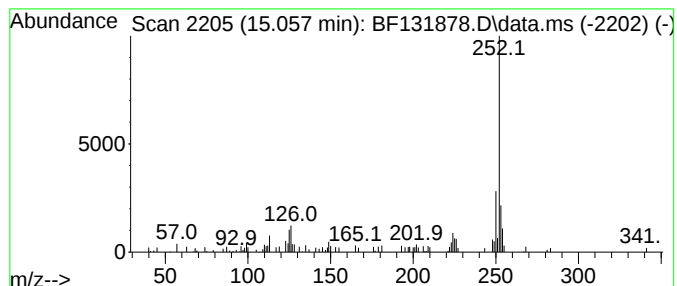
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[j]fluoranthene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.057	2.10 ng	45328	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	93
2			Benzo[j]fluoranthene	252	C20H12	000205-82-3	81
3			Perylene	252	C20H12	000198-55-0	81
4			Benzo[e]pyrene	252	C20H12	000192-97-2	81
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122922\
Data File : BF131878.D
Acq On : 29 Dec 2022 15:15
Operator : CG\JU
Sample : N6231-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

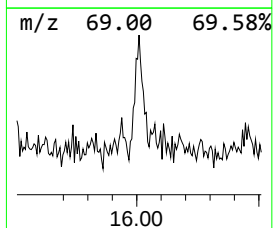
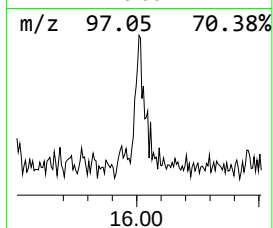
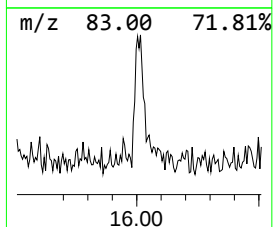
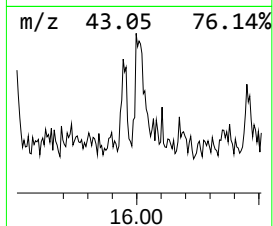
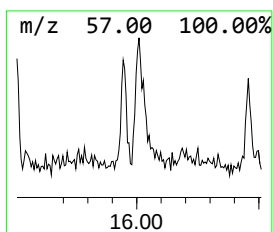
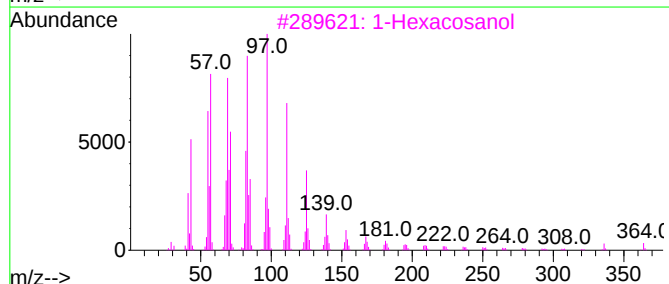
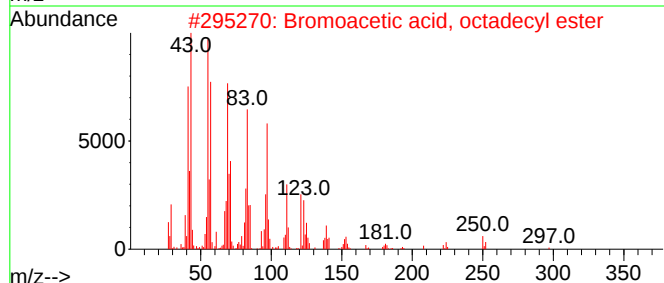
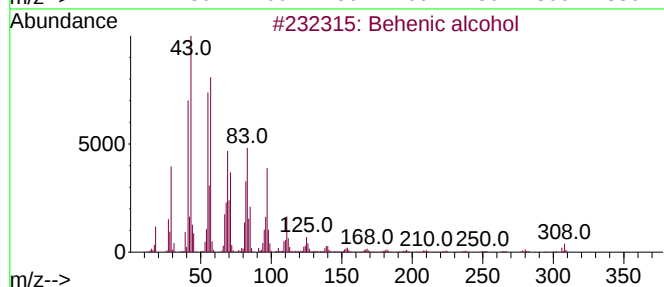
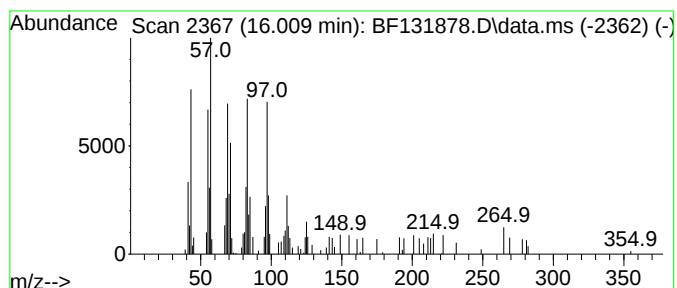
Instrument :
BNA_F
ClientSampleId :
TP-3S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Behenic alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.009	2.42 ng	52200	Perylene-d12	15.486	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	83
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	83
3	1-Hexacosanol	382	C26H54O	000506-52-5	68
4	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	64
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122922\
Data File : BF131878.D
Acq On : 29 Dec 2022 15:15
Operator : CG\JU
Sample : N6231-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.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
2-Pentanone, 4-...	5.034	41.0	ng	1013350	1	6.816	494355	20.0
Benzophenone	10.586	3.5	ng	136399	3	9.869	787641	20.0
n-Hexadecanoic ...	11.892	4.0	ng	160627	4	11.363	805392	20.0
Benzene, 1,1'-(...	12.804	3.0	ng	79025	5	14.010	530944	20.0
n-Tetracosanol-1	13.845	12.1	ng	320826	5	14.010	530944	20.0
Triphenylphosph...	14.110	8.8	ng	234368	5	14.010	530944	20.0
Benzo[j]fluoran...	15.057	2.1	ng	45328	6	15.486	431855	20.0
Behenic alcohol	16.009	2.4	ng	52200	6	15.486	431855	20.0