

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
 Data File : BF131026.D
 Acq On : 05 Nov 2022 18:46
 Operator : CG\JU
 Sample : N5318-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20221111-COMP-10

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131026.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	12	20	28	rVB	523969	690253	34.27%	4.795%
2	2.310	34	38	48	rVB	42796	55758	2.77%	0.387%
3	5.128	512	517	525	rBV	285402	356985	17.72%	2.480%
4	5.522	579	584	587	rBV	1973731	1863329	92.52%	12.944%
5	6.528	749	755	758	rBV	1820009	1848293	91.77%	12.839%
6	6.898	815	818	822	rBV	440488	386800	19.20%	2.687%
7	7.463	909	914	918	rBV	1075167	1119500	55.58%	7.777%
8	8.087	1016	1020	1033	rBV	28774	56695	2.81%	0.394%
9	8.187	1033	1037	1040	rBV	633785	514680	25.55%	3.575%
10	9.263	1215	1220	1223	rBV	2383471	2014063	100.00%	13.991%
11	9.945	1332	1336	1339	rBV	791328	622252	30.90%	4.323%
12	10.739	1466	1471	1474	rBV	1434147	1252672	62.20%	8.702%
13	11.439	1586	1590	1593	rBV	752245	595285	29.56%	4.135%
14	11.504	1596	1601	1604	rVB2	30083	23017	1.14%	0.160%
15	12.533	1771	1776	1779	rBV2	30704	26440	1.31%	0.184%
16	13.027	1856	1860	1863	rBV	1887660	1686759	83.75%	11.717%
17	13.986	2017	2023	2033	rBV7	19793	61555	3.06%	0.428%
18	14.086	2036	2040	2043	rVB	429901	373622	18.55%	2.595%
19	14.180	2051	2056	2063	rVB	65704	69498	3.45%	0.483%
20	15.139	2214	2219	2222	rBV	16839	25089	1.25%	0.174%
21	15.216	2228	2232	2237	rVB2	24227	30683	1.52%	0.213%
22	15.586	2289	2295	2305	rVB	380005	511551	25.40%	3.554%
23	16.063	2371	2376	2381	rBV	33326	50523	2.51%	0.351%
24	16.586	2460	2465	2472	rBV3	32007	65705	3.26%	0.456%
25	17.210	2565	2571	2578	rBV3	20881	41075	2.04%	0.285%
26	17.951	2691	2697	2707	rVB4	19865	53516	2.66%	0.372%

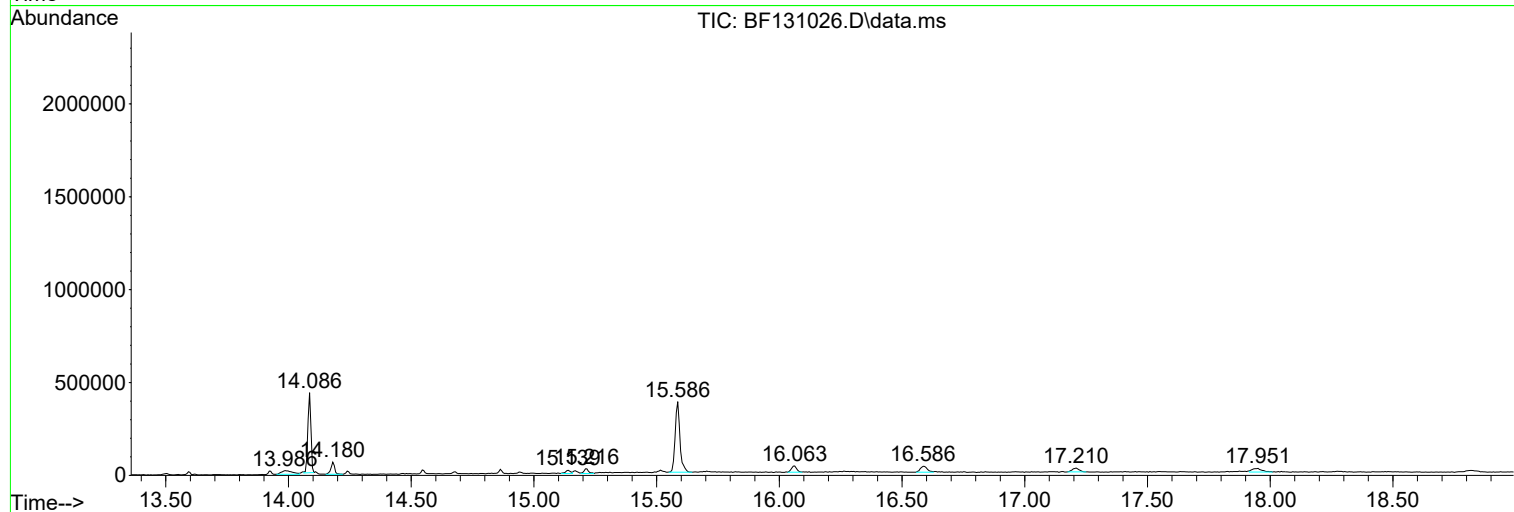
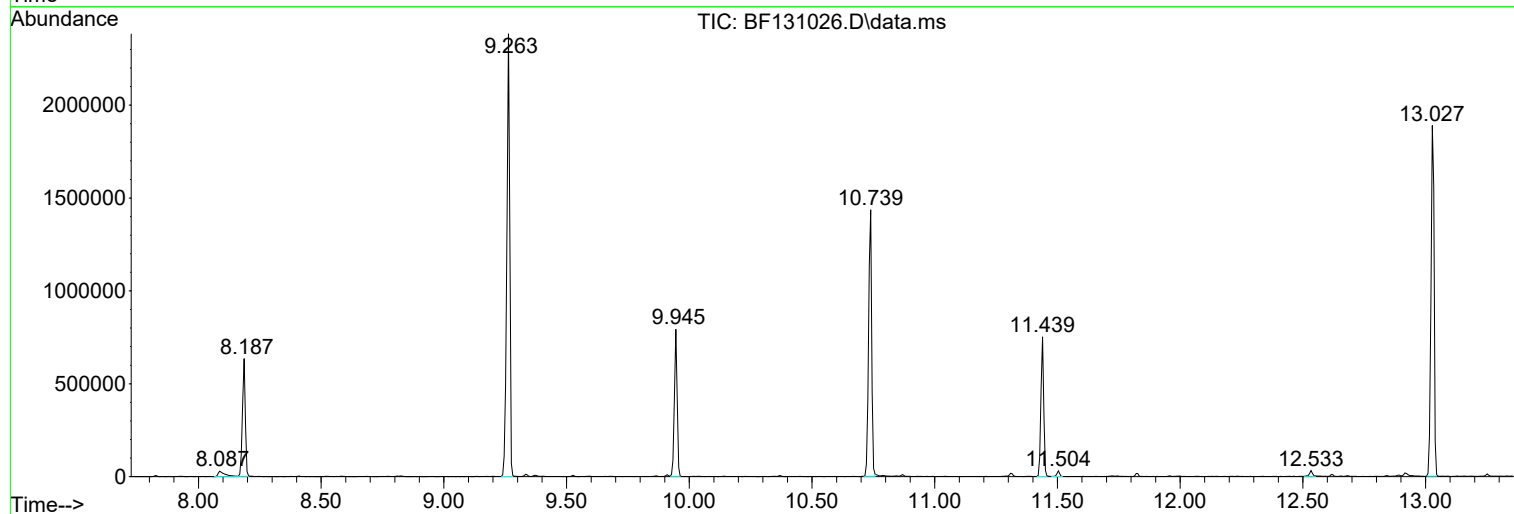
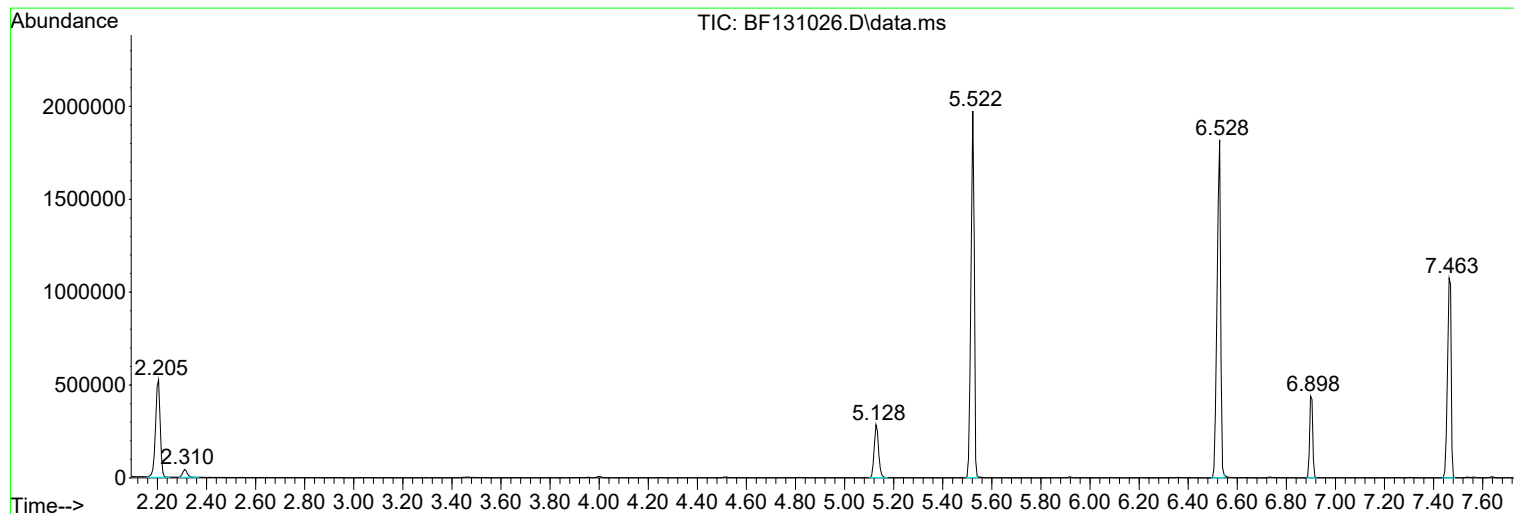
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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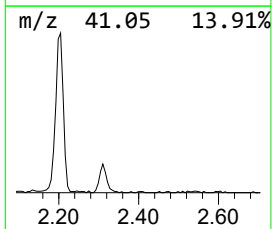
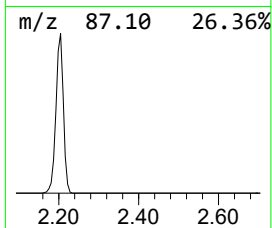
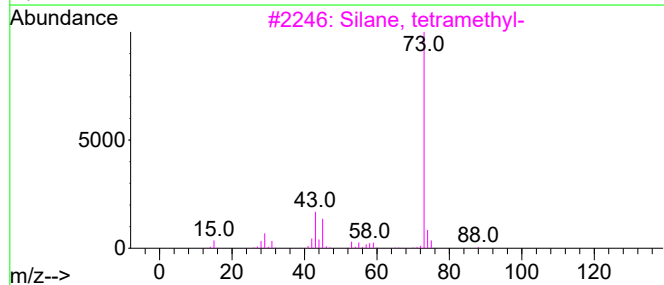
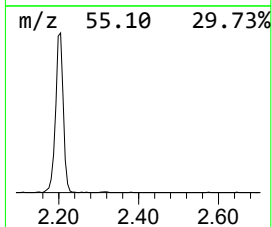
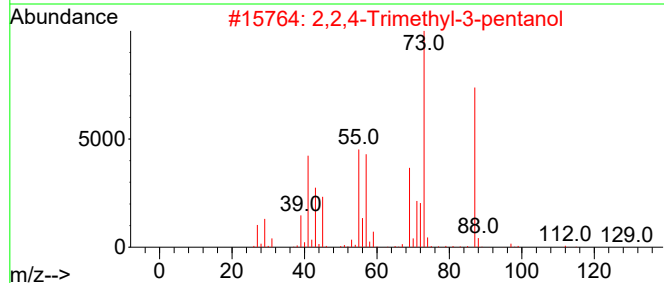
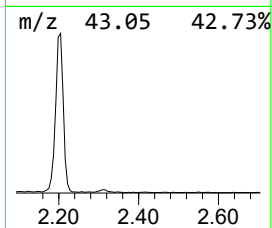
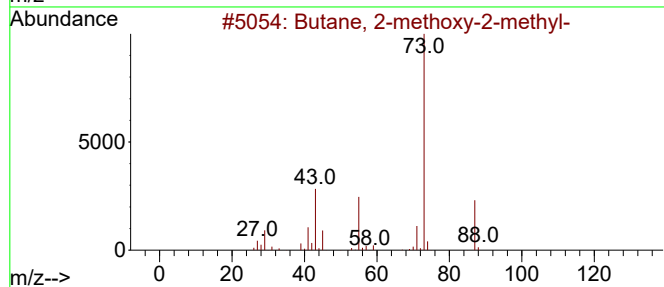
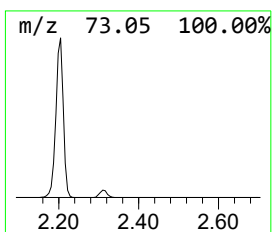
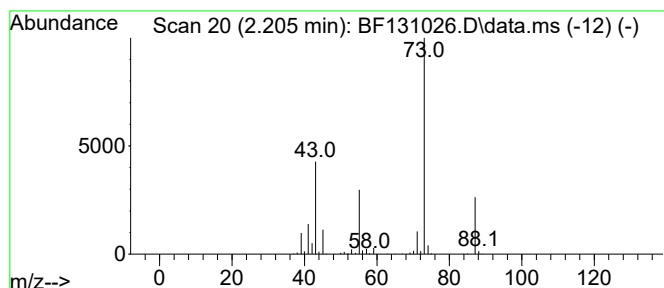
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.205	35.69 ng	690253	1,4-Dichlorobenzene-d4	6.904

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	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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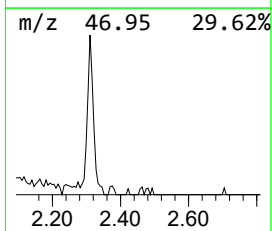
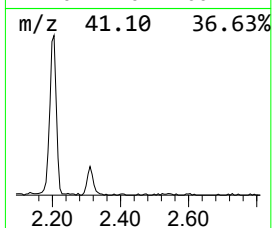
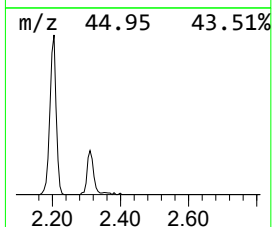
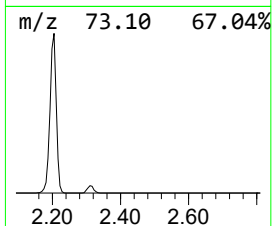
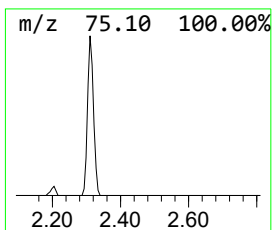
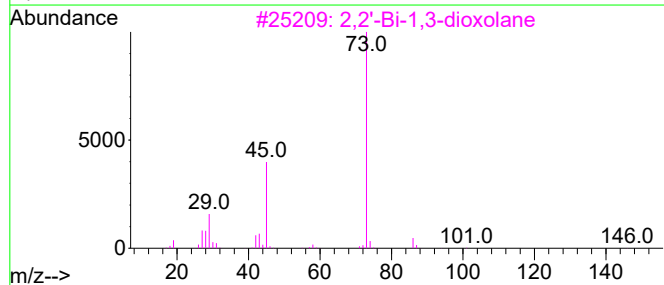
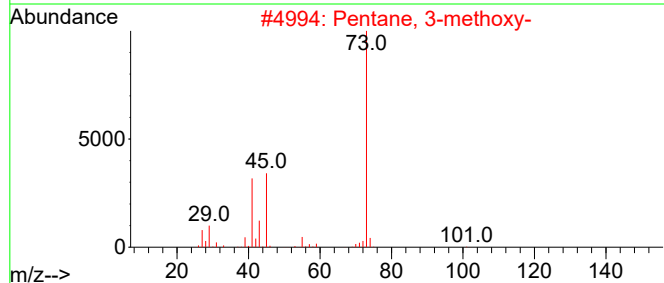
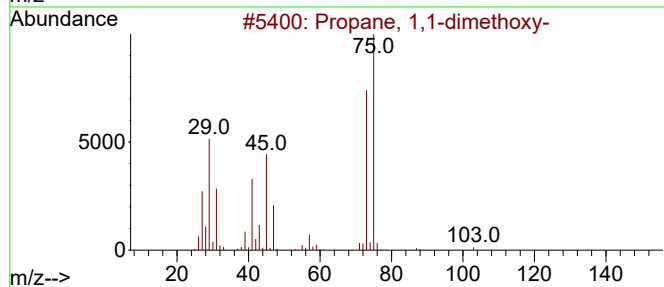
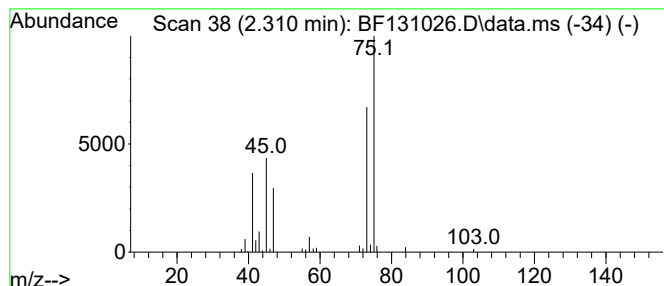
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.310	2.88 ng	55758	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
3			2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	12
4			3-Hexene, 1-(1-ethoxyethoxy)-, (Z)-	172	C10H20O2	028069-74-1	10
5			Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9



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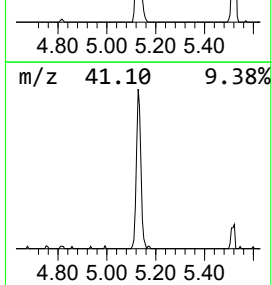
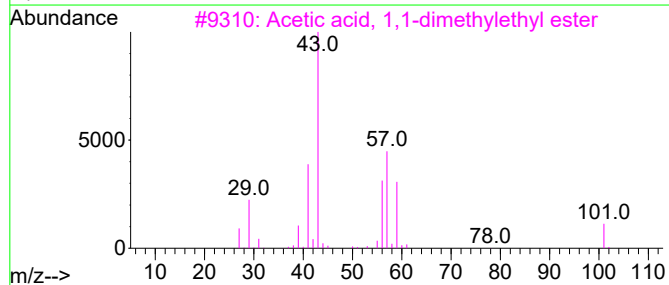
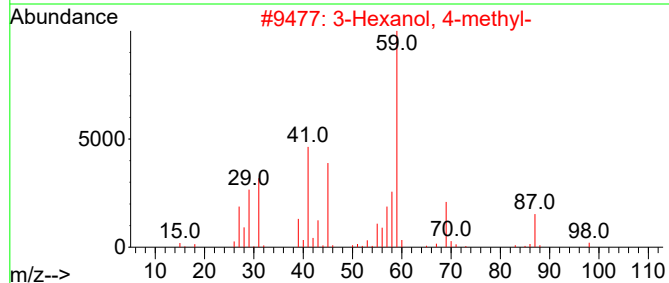
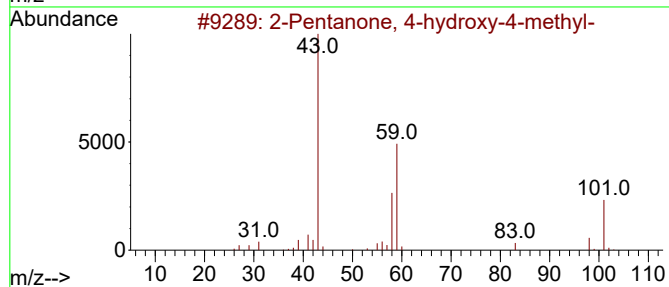
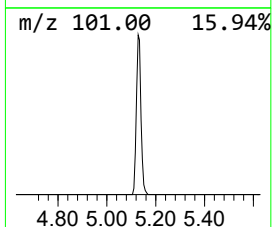
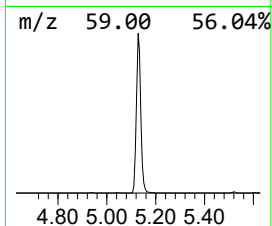
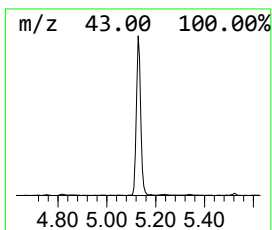
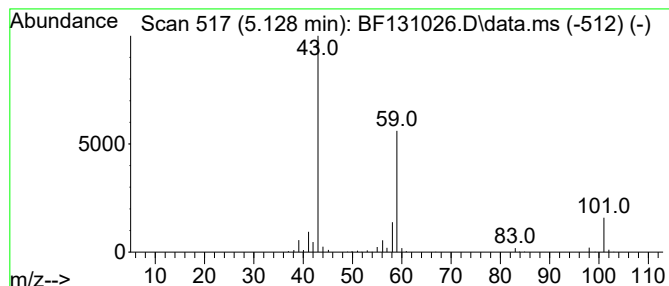
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	18.46 ng	356985	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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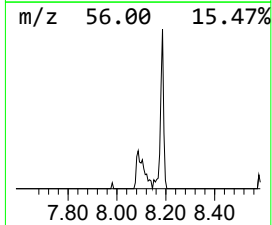
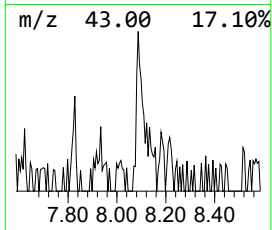
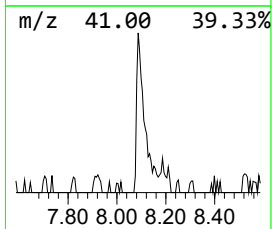
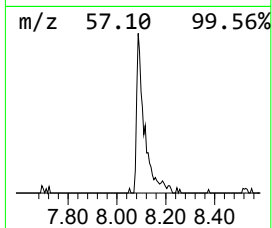
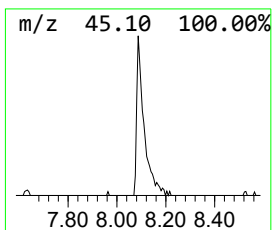
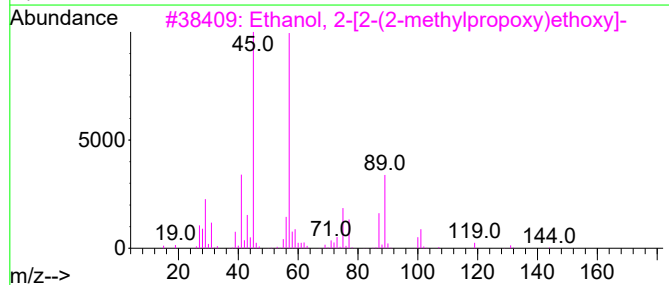
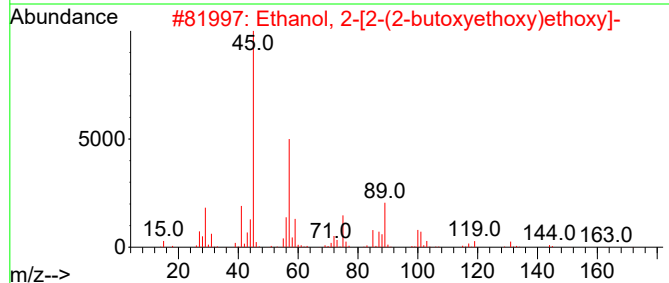
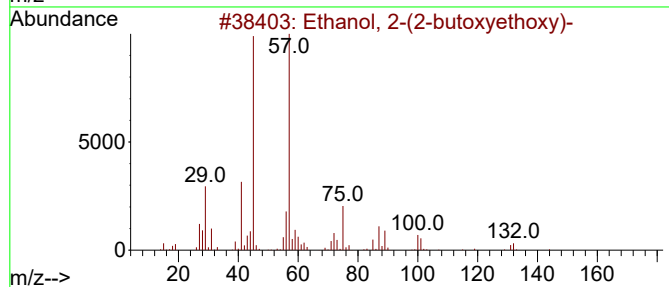
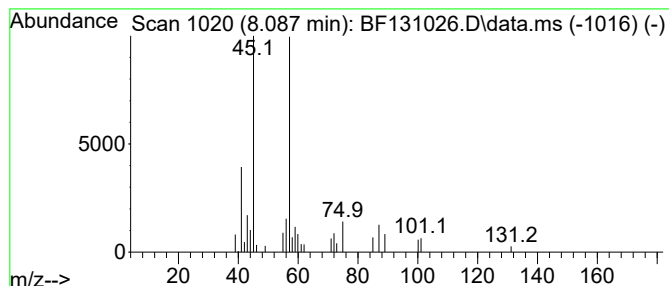
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.087	2.20 ng	56695	Naphthalene-d8	8.187

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	64
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	50
5			Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	50



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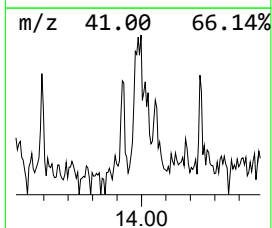
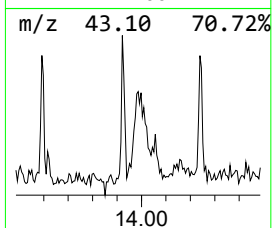
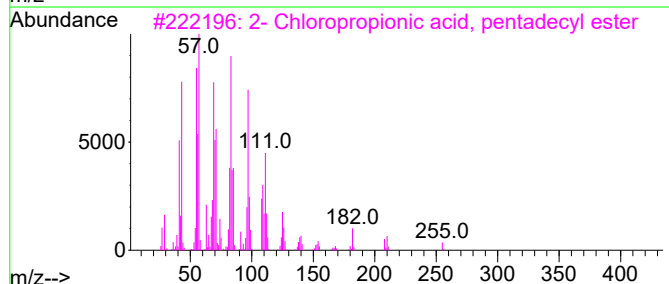
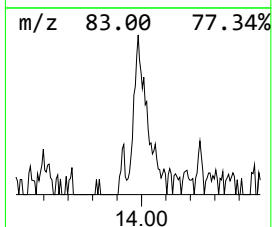
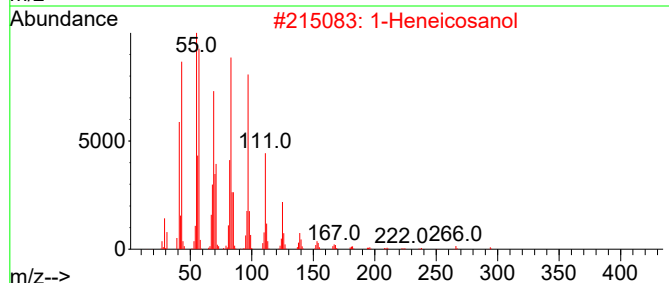
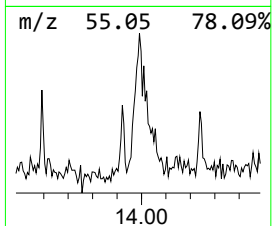
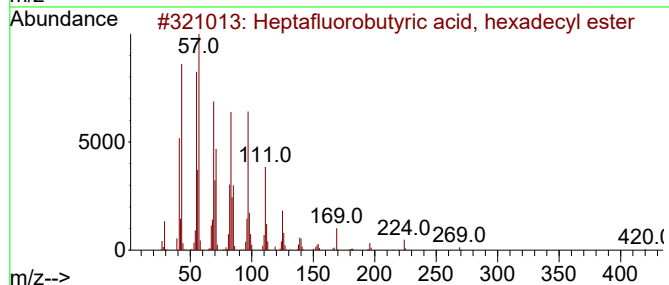
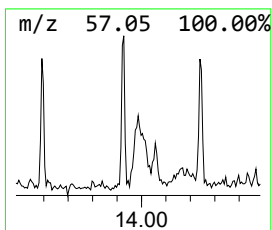
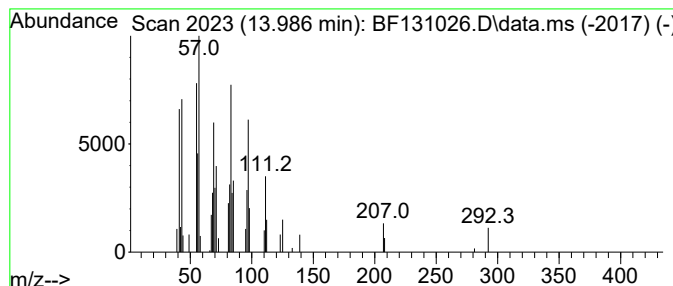
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptafluorobutyric acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.986	3.30 ng	61555	Chrysene-d12	14.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90
2			1-Heneicosanol	312	C21H44O	015594-90-8	90
3			2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	90
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	90



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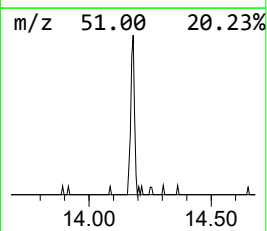
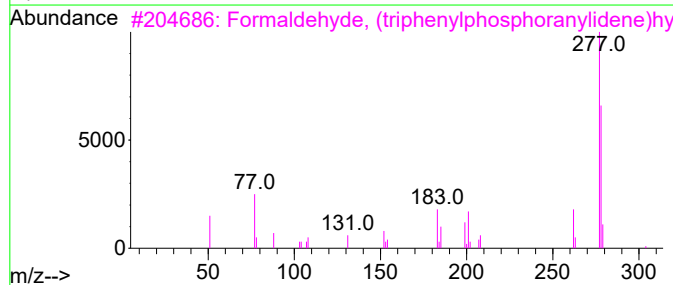
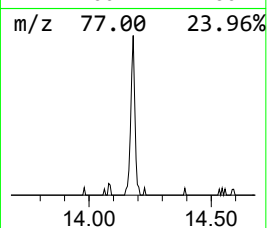
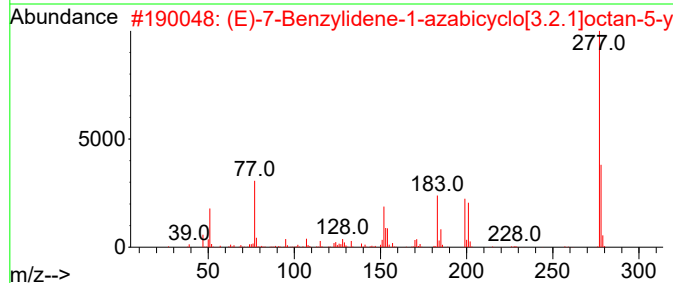
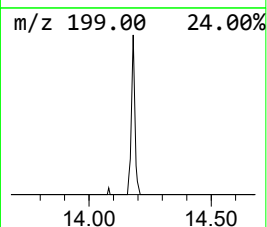
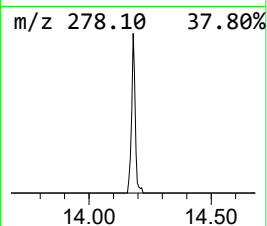
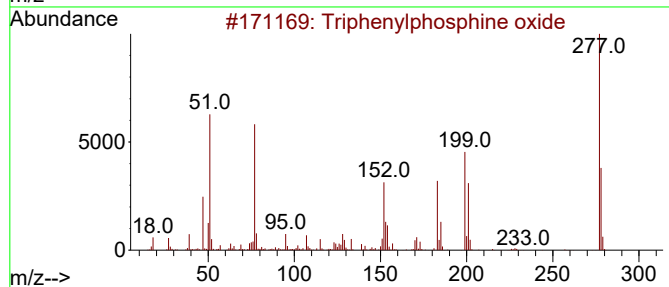
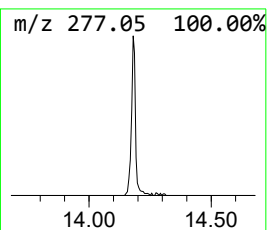
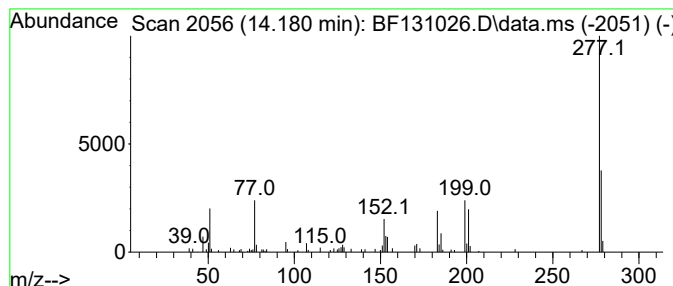
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
14.180	3.72 ng	69498	Chrysene-d12	14.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	99
2			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	90
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	23
5			1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19NO3Si	072101-35-0	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131026.D
Acq On : 05 Nov 2022 18:46
Operator : CG\JU
Sample : N5318-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221111-COMP-10

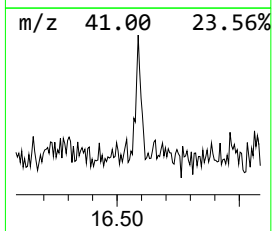
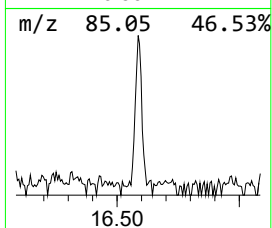
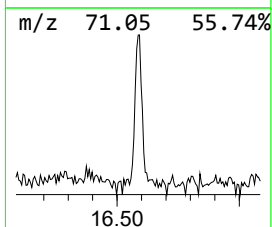
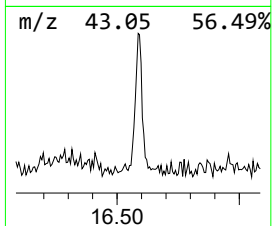
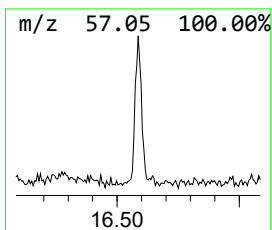
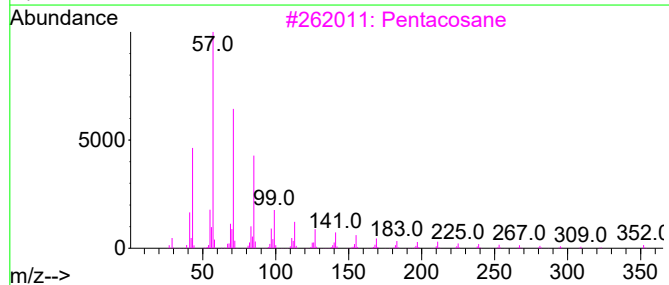
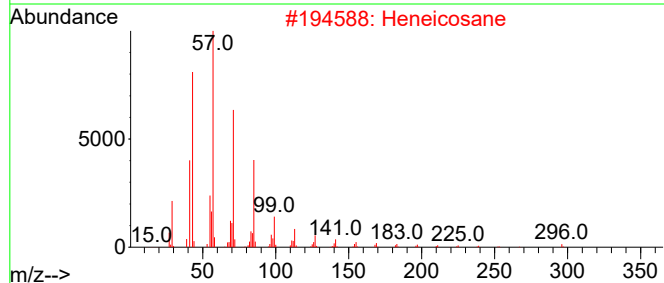
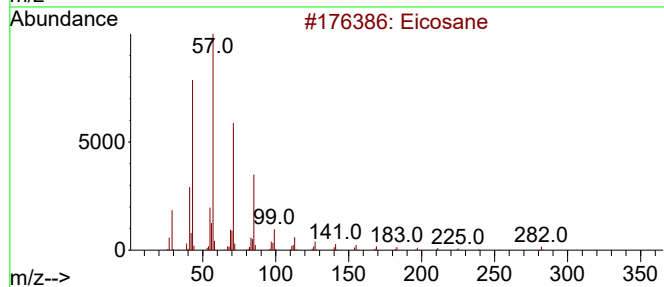
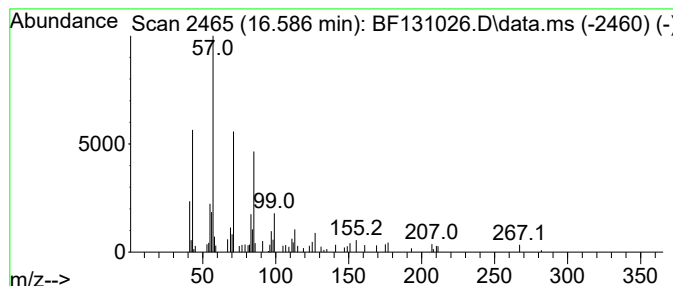
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.586	2.57 ng	65705	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	87
2	Heneicosane			296	C21H44	000629-94-7	86
3	Pentacosane			352	C25H52	000629-99-2	86
4	Hentriacontane			437	C31H64	000630-04-6	86
5	Octadecane			254	C18H38	000593-45-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131026.D
Acq On : 05 Nov 2022 18:46
Operator : CG\JU
Sample : N5318-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221111-COMP-10

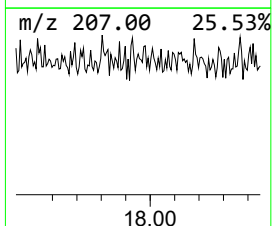
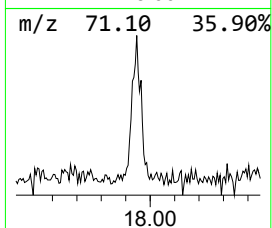
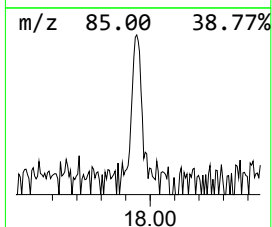
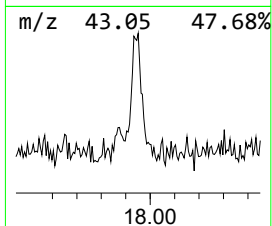
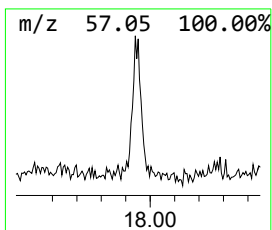
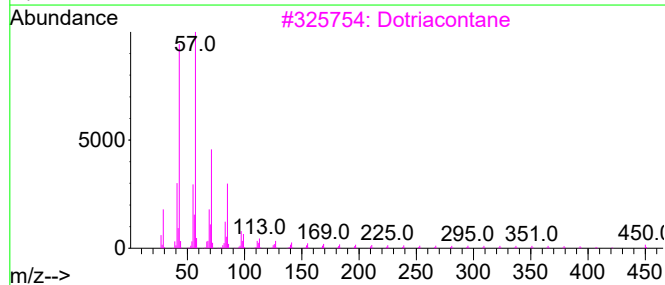
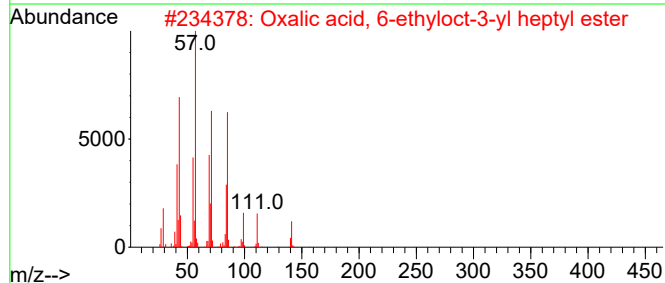
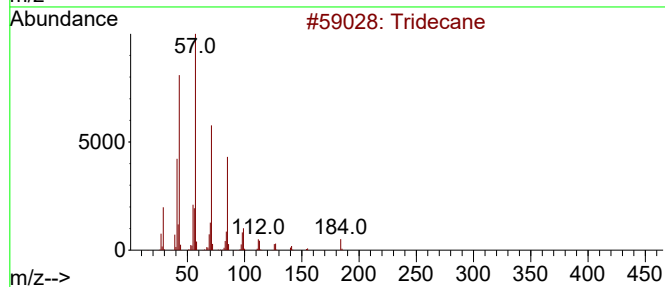
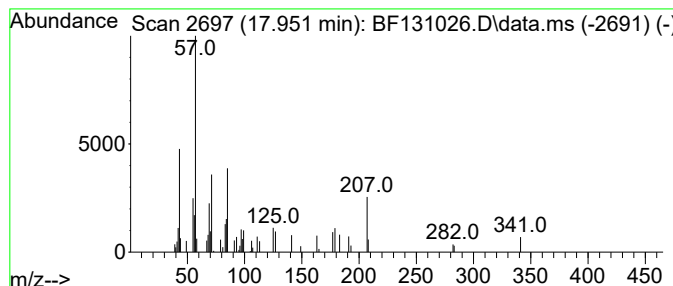
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown17.951 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.951	2.09 ng	53516	Perylene-d12	15.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	27
2			Oxalic acid, 6-ethyloct-3-yl hep...	328	C19H36O4	1000309-34-5	27
3			Dotriacontane	451	C32H66	000544-85-4	27
4			Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	27
5			Oxalic acid, bis(6-ethyloct-3-yl...	370	C22H42O4	1000309-34-6	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110522\
Data File : BF131026.D
Acq On : 05 Nov 2022 18:46
Operator : CG\JU
Sample : N5318-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221111-COMP-10

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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...	2.205	35.7	ng	690253	1	6.904	386800	20.0
Propane, 1,1-di...	2.310	2.9	ng	55758	1	6.904	386800	20.0
2-Pentanone, 4-...	5.128	18.5	ng	356985	1	6.904	386800	20.0
Ethanol, 2-(2-b...	8.087	2.2	ng	56695	2	8.187	514680	20.0
Heptafluorobuty...	13.986	3.3	ng	61555	5	14.086	373622	20.0
Triphenylphosph...	14.180	3.7	ng	69498	5	14.086	373622	20.0
Eicosane	16.586	2.6	ng	65705	6	15.586	511551	20.0
unknown17.951	17.951	2.1	ng	53516	6	15.586	511551	20.0