LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF131004.D
Acq On : 04 Nov 2022 22:31
Operator : CG\JU
Sample : N5318-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221105-COMP-04

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: BF131004.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	26	rVB	401878	522136	21.72%	3.368%
2	2.316	33	39	45	rVB	39930	51226	2.13%	0.330%
3	5.140	514	519	529	rBV	314876	376809	15.67%	2.430%
4	5.534	581	586	589	rBV	2247814	2103323	87.49%	13.566%
5	6.534	751	756	759	rBV	2027424	2175701	90.50%	14.033%
6	6.910	816	820	823	rBV	572308	440686	18.33%	2.842%
7	7.475	911	916	919	rBV	1597823	1496437	62.25%	9.652%
8	8.092	1018	1021	1034	rBV	197499	292757	12.18%	1.888%
9	8.192	1034	1038	1042	rVB	672480	608595	25.32%	3.925%
10	9.275	1216	1222	1225	rBV	2743930	2403976	100.00%	15.506%
11	9.957	1333	1338	1341	rVB	763492	644615	26.81%	4.158%
12	10.745	1468	1472	1479	rBV	1161103	993912	41.34%	6.411%
13	10.869	1487	1493	1500	rVB7	16159	34834	1.45%	0.225%
14	11.328	1567	1571	1578	rVB6	18049	29361	1.22%	0.189%
15	11.445	1588	1591	1595	rBV	604981	535668	22.28%	3.455%
16	12.892	1832	1837	1844	rBV	32713	44133	1.84%	0.285%
17	13.039	1858	1862	1865	rBV	1974010	1690900	70.34%	10.906%
18	14.016	2019	2028	2035	rBV	21086	76697	3.19%	0.495%
19	14.098	2038	2042	2045	rBV	511422	453544	18.87%	2.925%
20	14.192	2053	2058	2062	rBV	90359	95233	3.96%	0.614%
21	14.957	2184	2188	2193	rBV2	18598	26999	1.12%	0.174%
22	15.604	2292	2298	2309	rBV	300521	406467	16.91%	2.622%

Sum of corrected areas: 15504009

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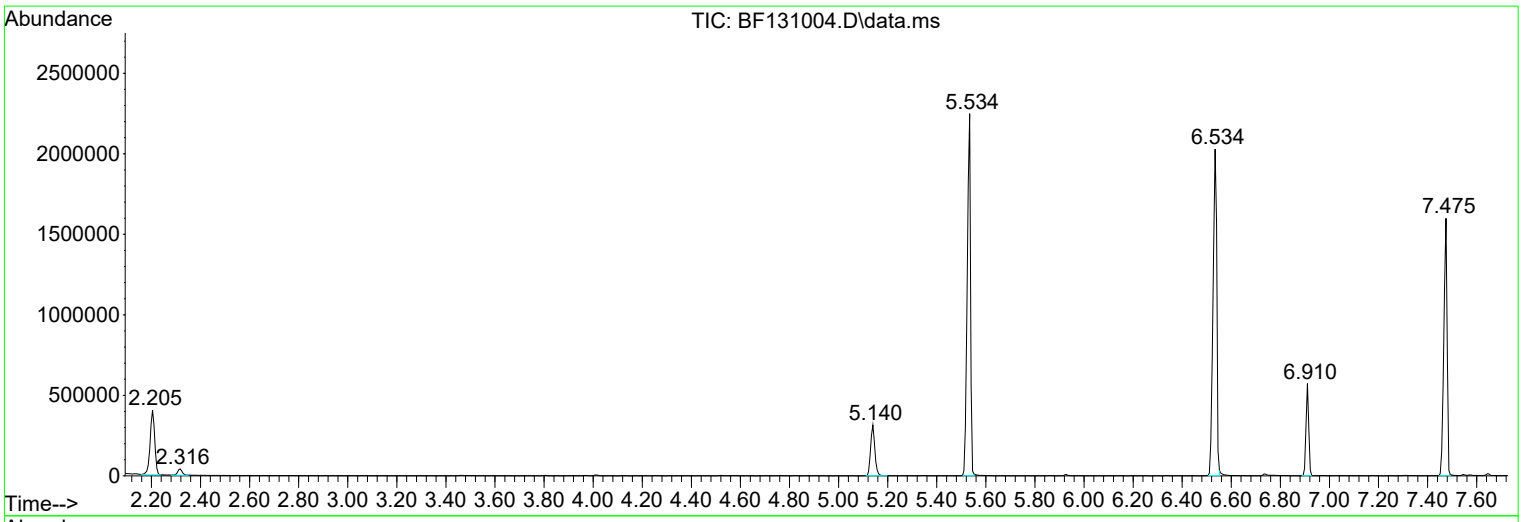
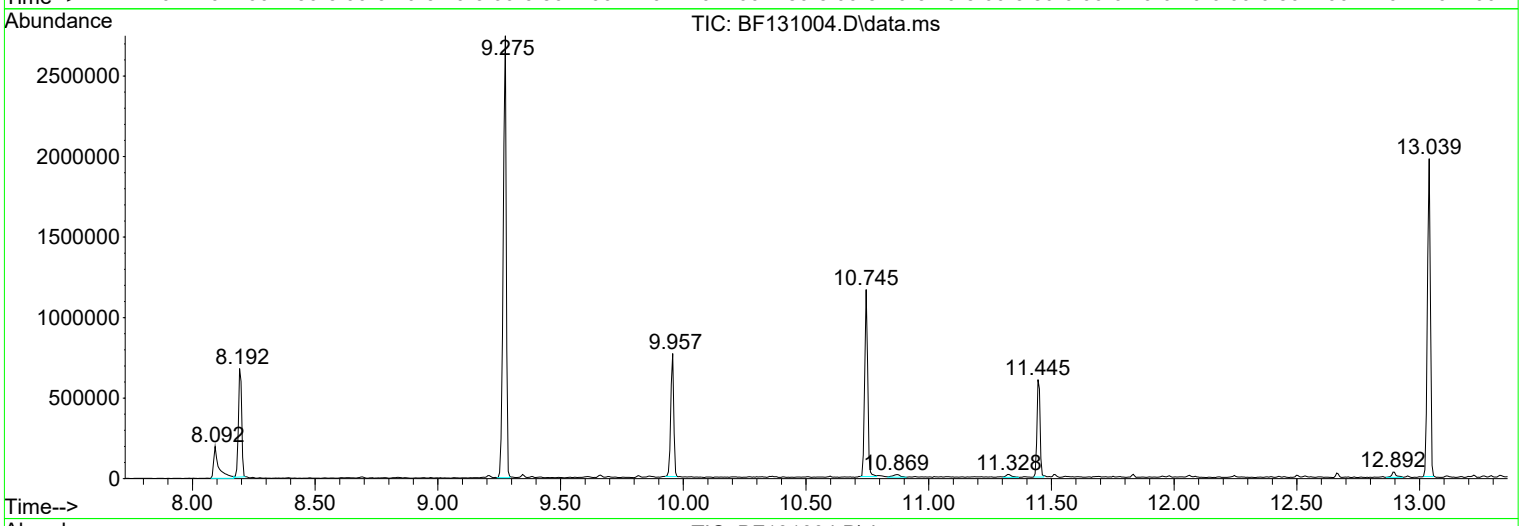
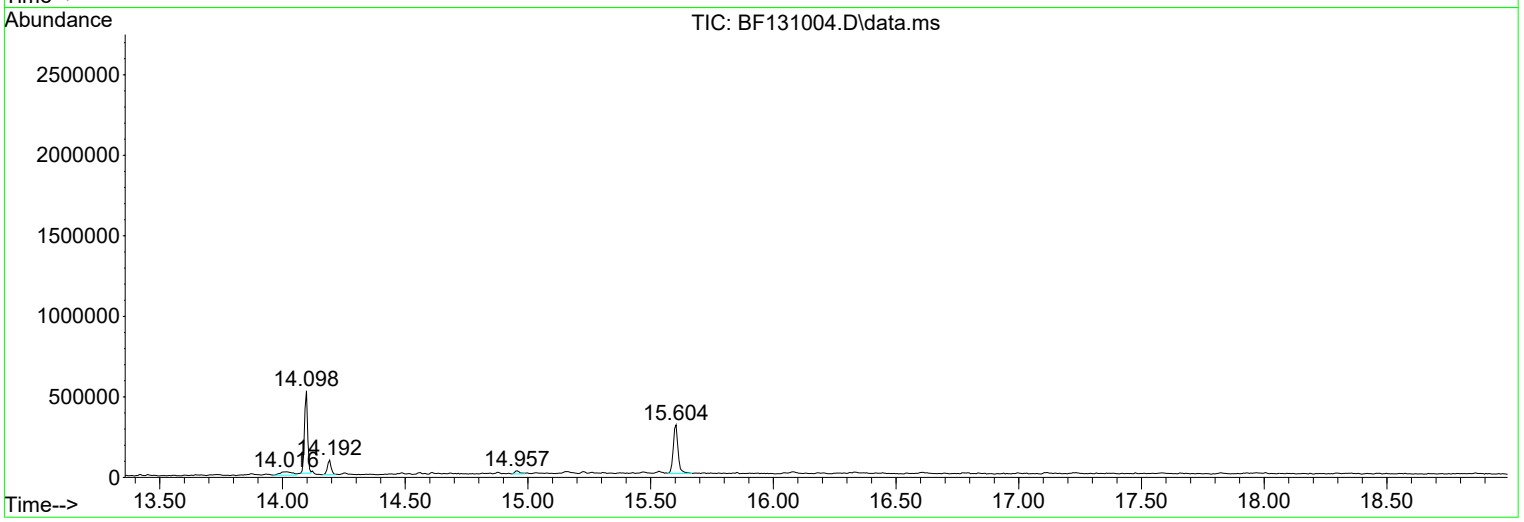
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

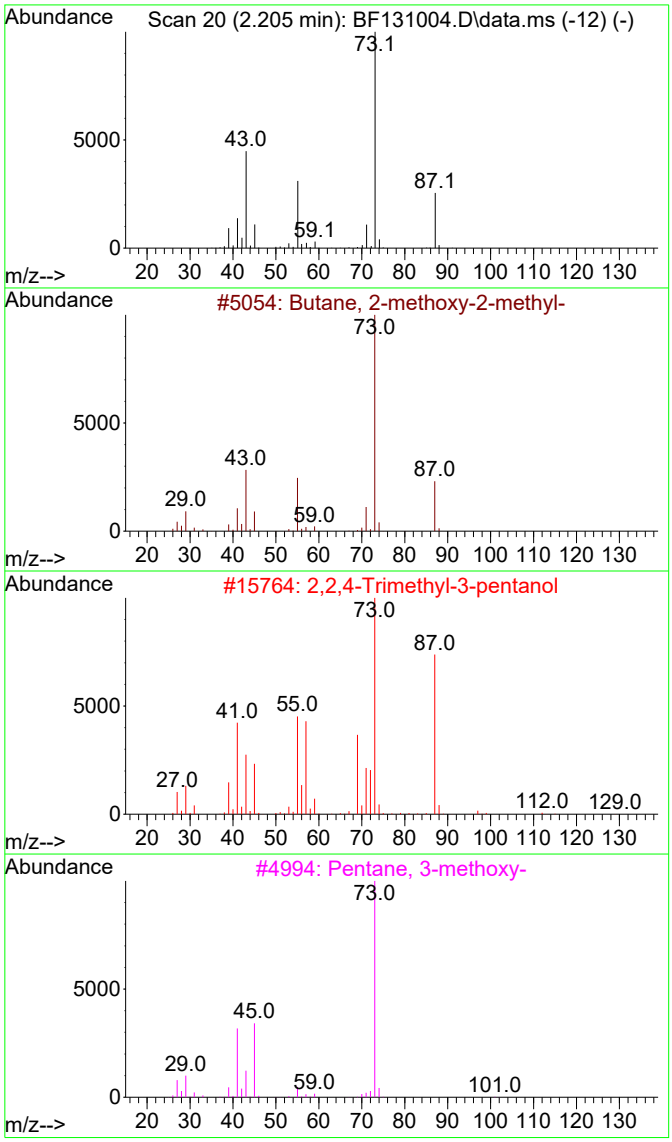
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

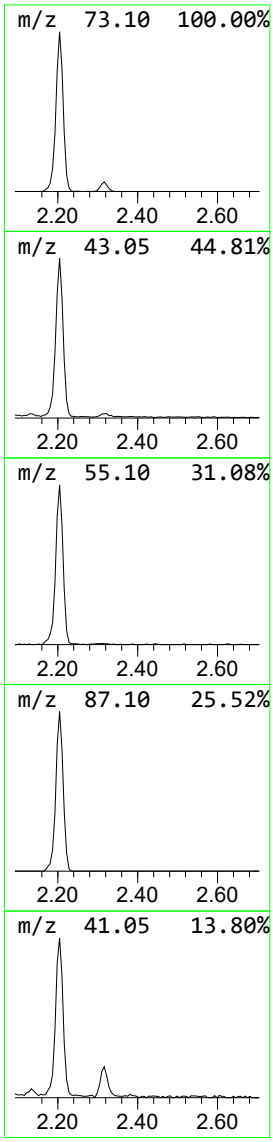
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.205	23.70 ng	522136	1,4-Dichlorobenzene-d4	6.910

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	38
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Instrument :
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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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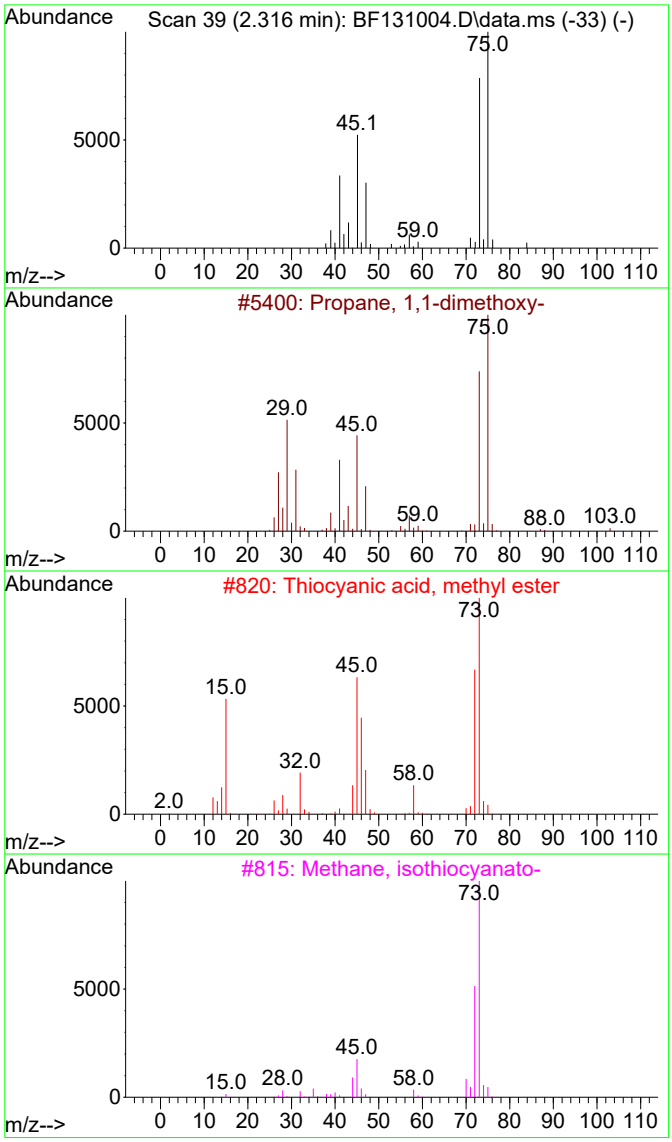
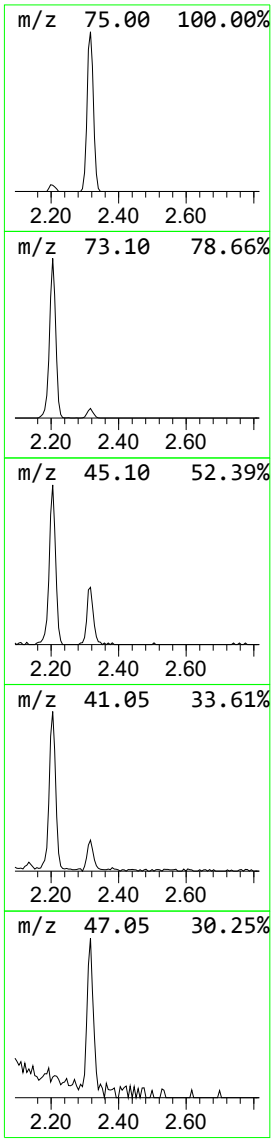
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.316	2.32 ng	51226	1,4-Dichlorobenzene-d4	6.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
3	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
4	1,2,4-Butanetriol	106	C4H10O3	003068-00-6	9
5	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9





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Operator : CG\JU
Sample : N5318-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221105-COMP-04

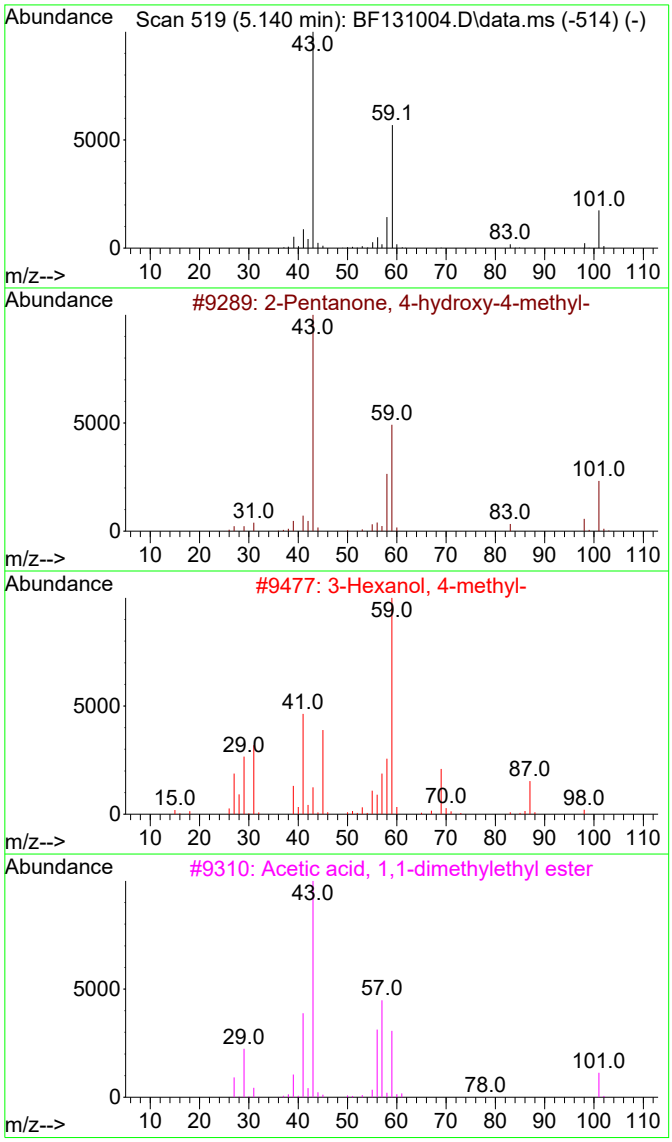
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

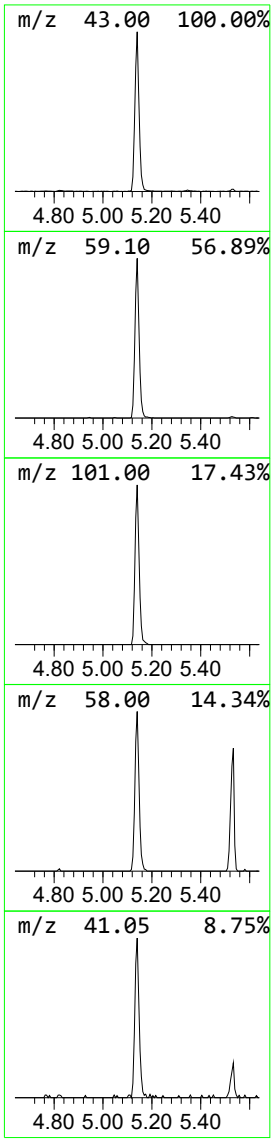
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.140	17.10 ng	376809	1,4-Dichlorobenzene-d4	6.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
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	10





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Sample : N5318-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221105-COMP-04

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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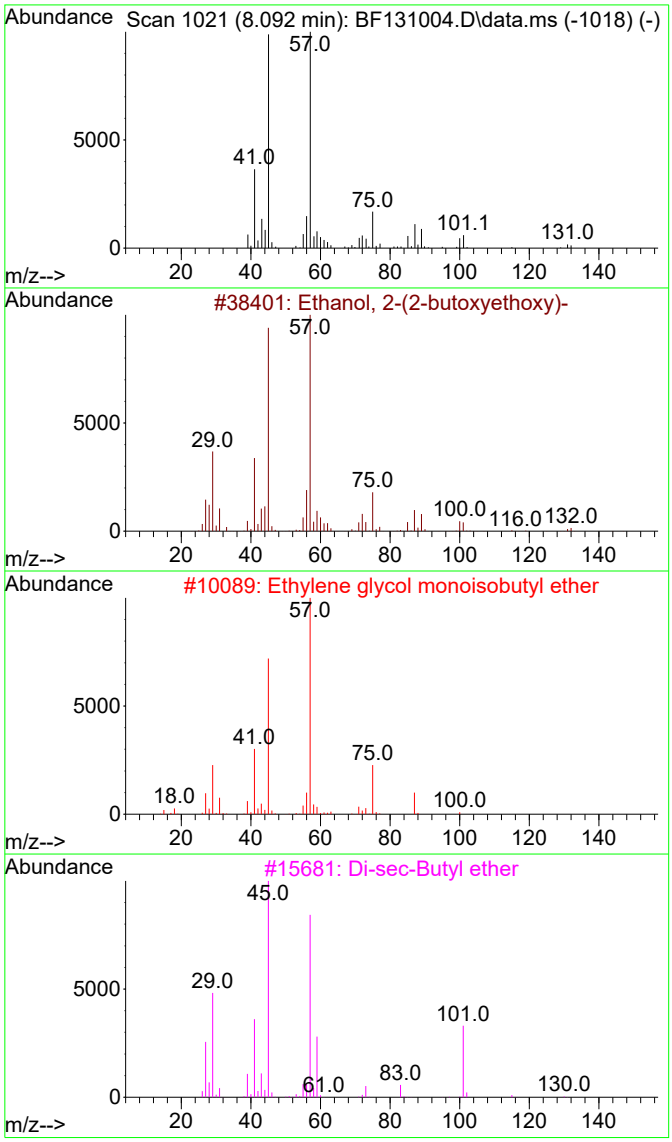
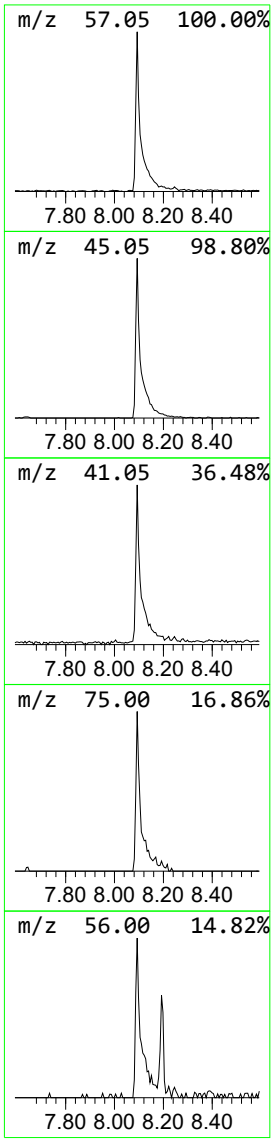
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	9.62 ng	292757	Naphthalene-d8	8.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
4	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	53
5	Butyl lactate	146	C7H14O3	000138-22-7	50





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Sample : N5318-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20221105-COMP-04

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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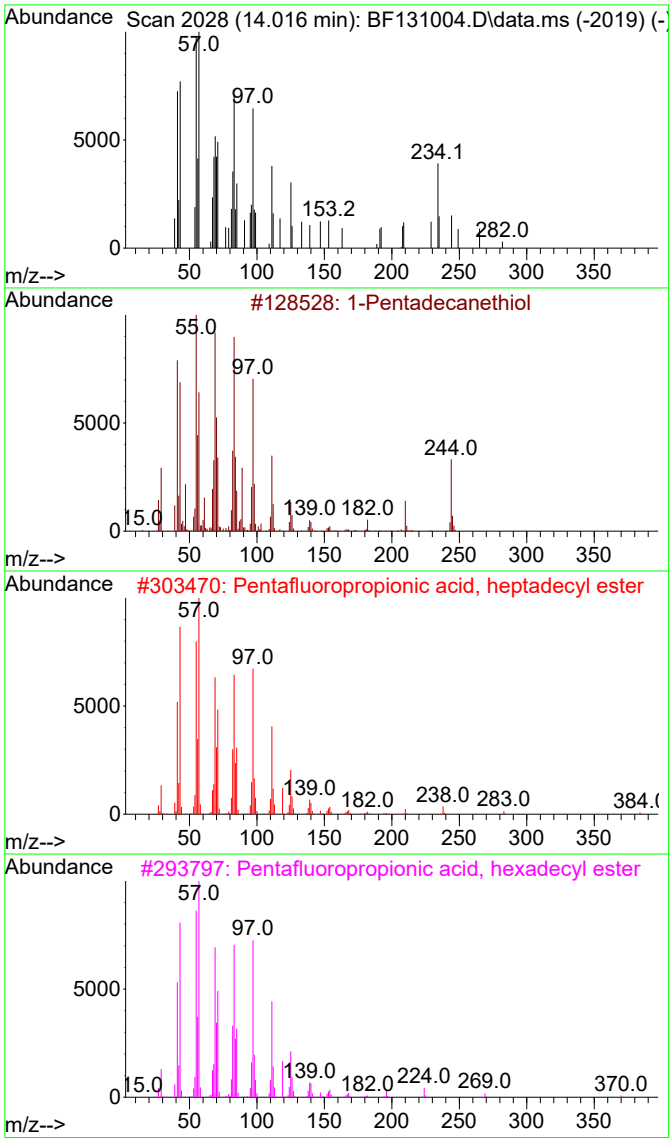
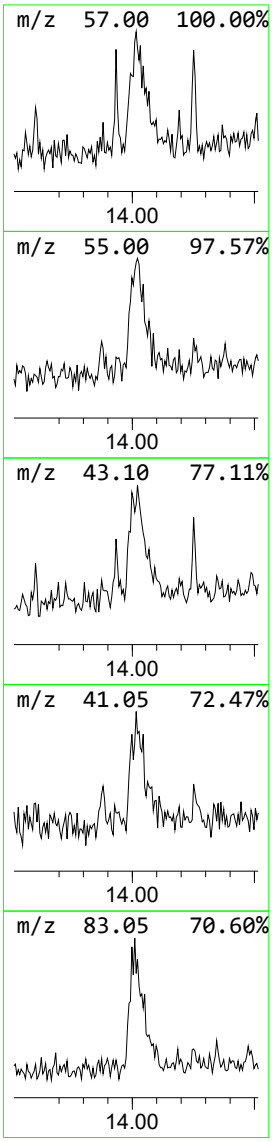
Peak Number 5 1-Pentadecanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.016	3.38 ng	76697	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecanethiol	244	C15H32S	025276-70-4	64
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	50
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	46
4	Octacosyl acetate	452	C30H60O2	018206-97-8	46
5	Octacosanol	410	C28H58O	000557-61-9	46





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Instrument :
BNA_F
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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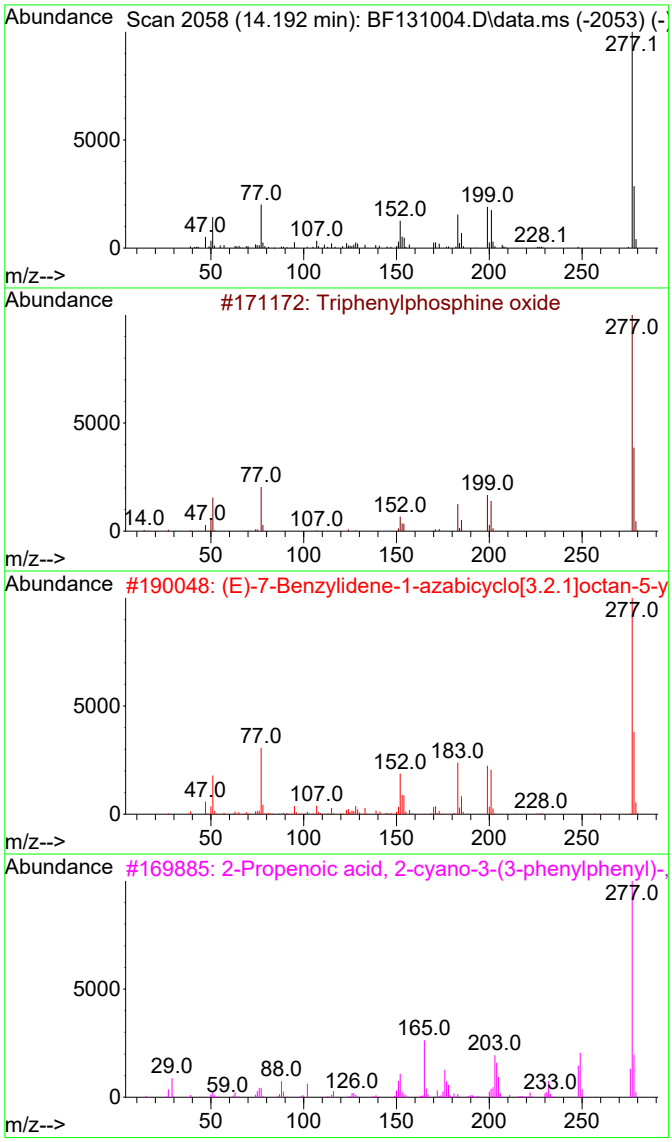
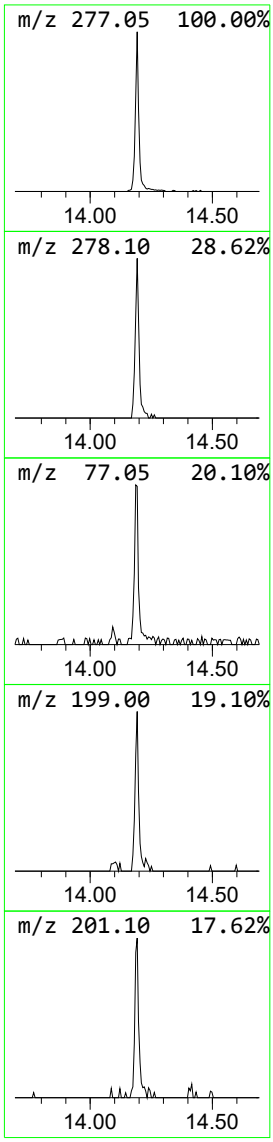
Peak Number 6 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	4.20 ng	95233	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15NO2	1000080-00-3	50
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	47
5	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.205	23.7	ng	522136	1	6.910	440686	20.0
Propane, 1,1-di...	2.316	2.3	ng	51226	1	6.910	440686	20.0
2-Pentanone, 4-...	5.140	17.1	ng	376809	1	6.910	440686	20.0
Ethanol, 2-(2-b...	8.092	9.6	ng	292757	2	8.192	608595	20.0
1-Pentadecanethiol	14.016	3.4	ng	76697	5	14.098	453544	20.0
Triphenylphosph...	14.192	4.2	ng	95233	5	14.098	453544	20.0