LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131131.D
Acq On : 10 Nov 2022 19:37
Operator : CG\JU
Sample : N5491-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

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-BF110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131131.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	9	17	23	rVB	394733	496491	21.85%	3.379%
2	2.299	31	36	43	rBV	34805	46622	2.05%	0.317%
3	4.493	406	409	416	rBV	56744	63195	2.78%	0.430%
4	5.116	510	515	525	rVB	417867	500937	22.04%	3.410%
5	5.510	578	582	585	rBV	2088119	1924552	84.68%	13.100%
6	6.516	748	753	756	rBV	2023079	1959946	86.24%	13.341%
7	6.887	813	816	820	rBV	582428	451482	19.87%	3.073%
8	7.451	907	912	915	rBV	1332156	1291117	56.81%	8.788%
9	8.169	1030	1034	1038	rBV	663420	583225	25.66%	3.970%
10	9.251	1213	1218	1221	rBV	2536464	2272700	100.00%	15.469%
11	9.933	1329	1334	1337	rBV	713031	637625	28.06%	4.340%
12	10.722	1464	1468	1479	rBV	1372528	1217767	53.58%	8.289%
13	11.422	1584	1587	1590	rBV	713737	587806	25.86%	4.001%
14	11.810	1649	1653	1656	rVB	53961	46492	2.05%	0.316%
15	12.869	1828	1833	1837	rBV	28397	30499	1.34%	0.208%
16	13.010	1853	1857	1861	rBV	1567354	1486696	65.42%	10.119%
17	13.974	2014	2021	2022	rBV6	24078	39636	1.74%	0.270%
18	14.074	2034	2038	2041	rBV	455911	415833	18.30%	2.830%
19	14.168	2049	2054	2057	rBV	59210	66220	2.91%	0.451%
20	14.827	2163	2166	2173	rBV2	42453	57388	2.53%	0.391%
21	14.921	2179	2182	2186	rVB	49087	48492	2.13%	0.330%
22	15.568	2287	2292	2301	rBV	379357	466963	20.55%	3.178%

Sum of corrected areas: 14691684

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
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Misc :
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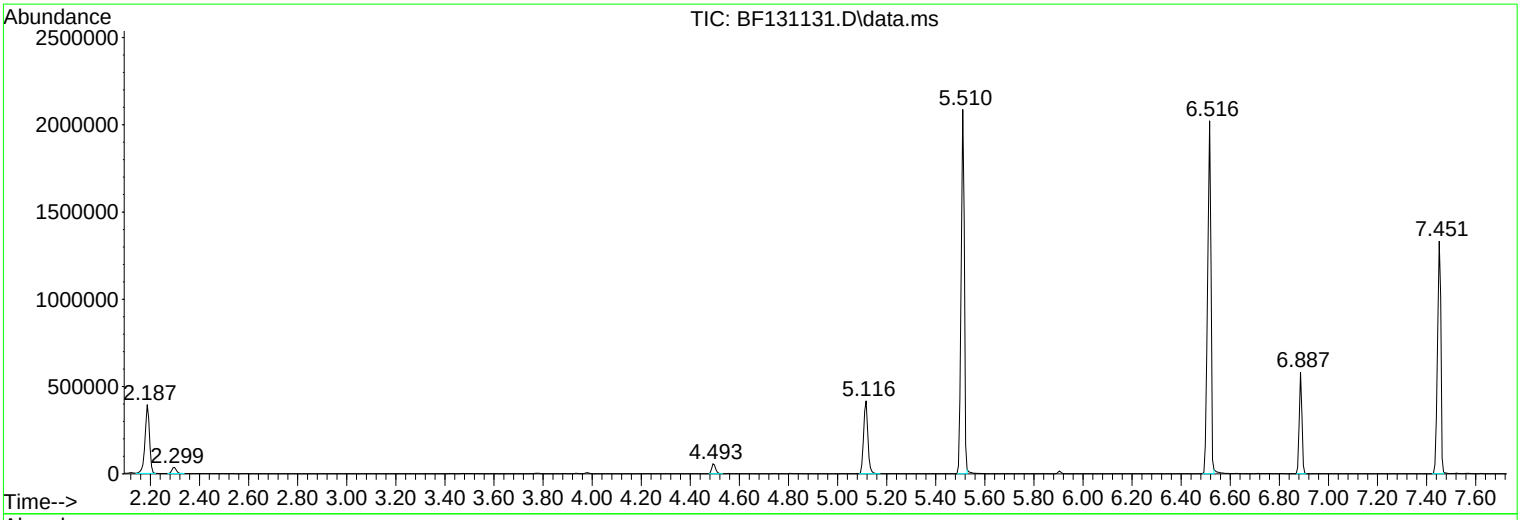
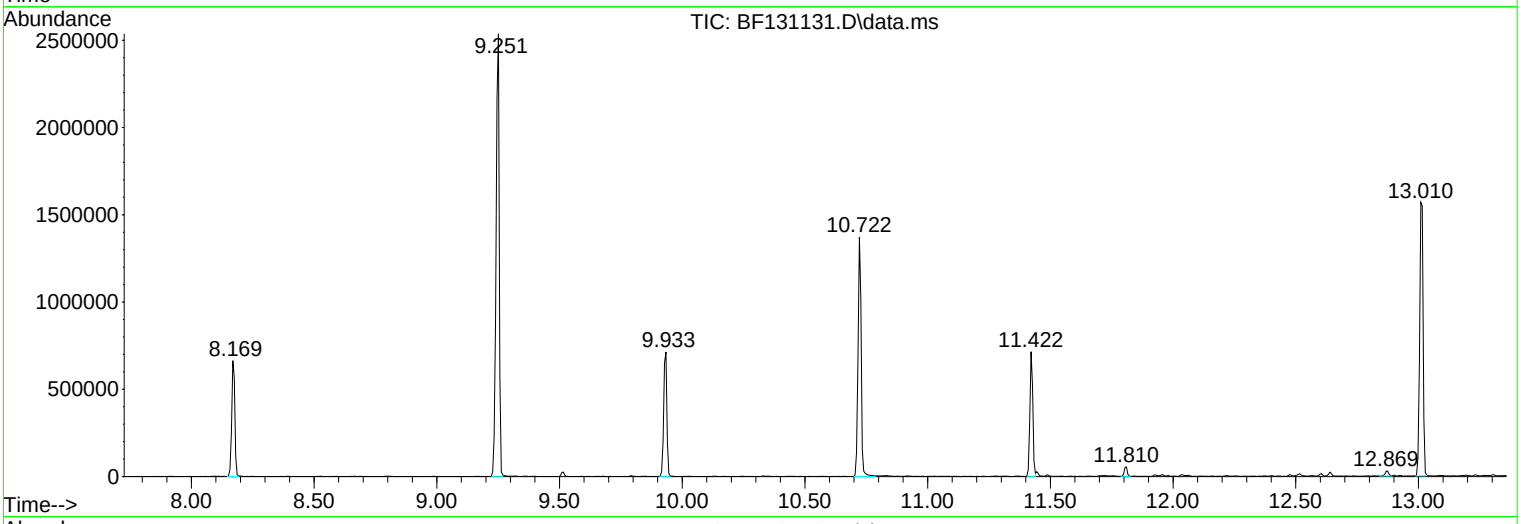
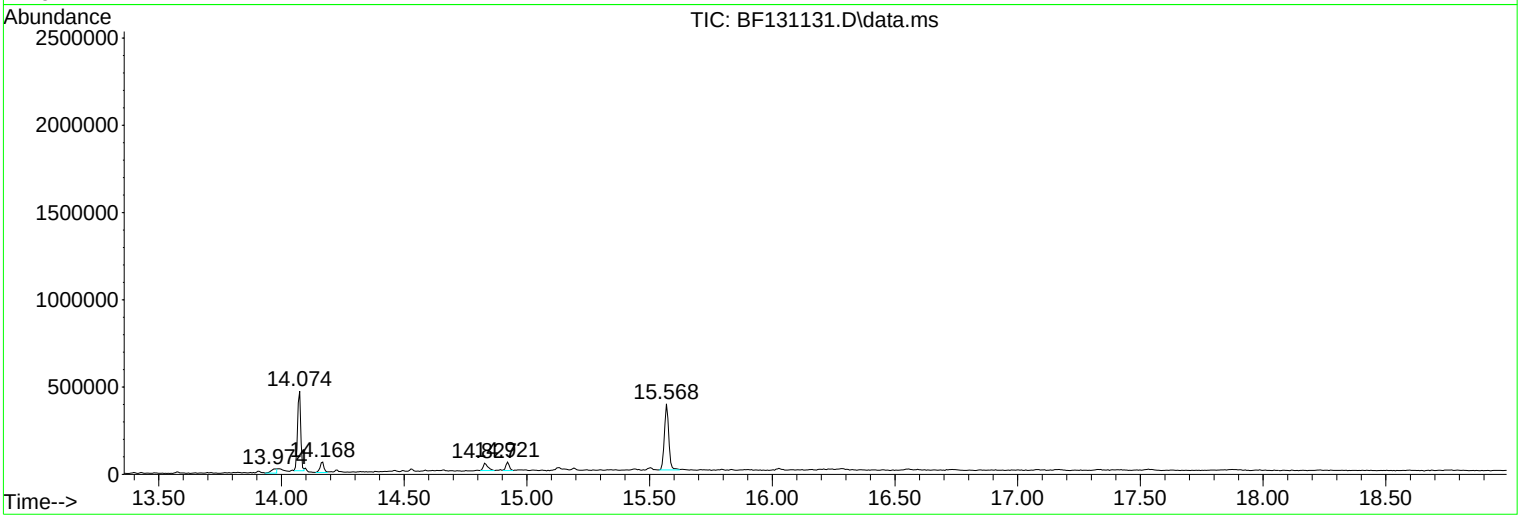
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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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Data File : BF131131.D
Acq On : 10 Nov 2022 19:37
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

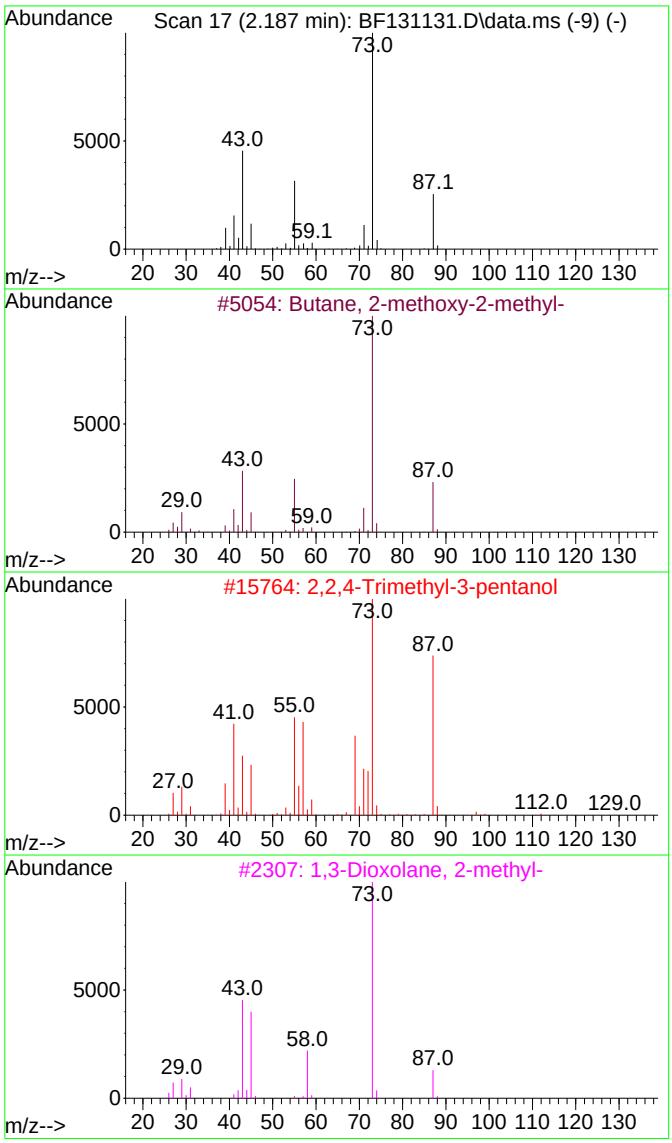
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

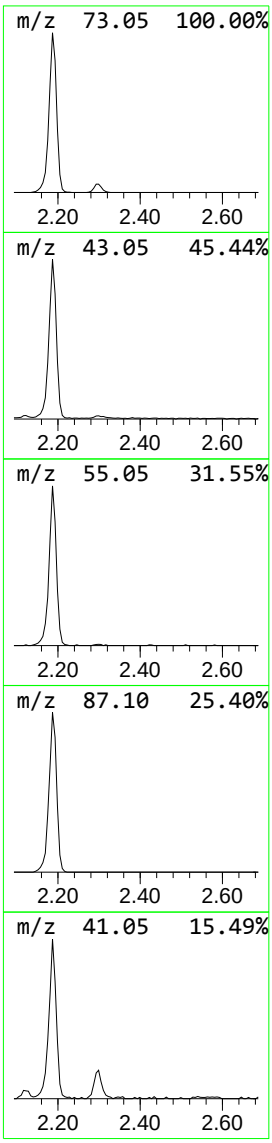
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	21.99 ng	496491	1,4-Dichlorobenzene-d4	6.887

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Data File : BF131131.D
Acq On : 10 Nov 2022 19:37
Operator : CG\JU
Sample : N5491-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

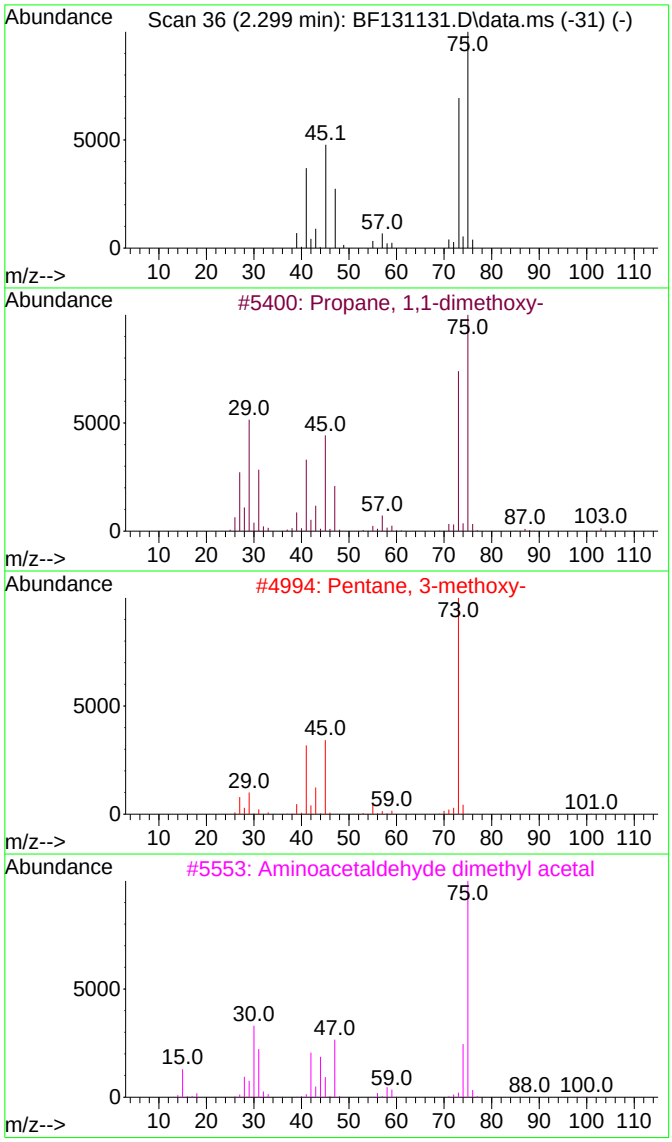
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

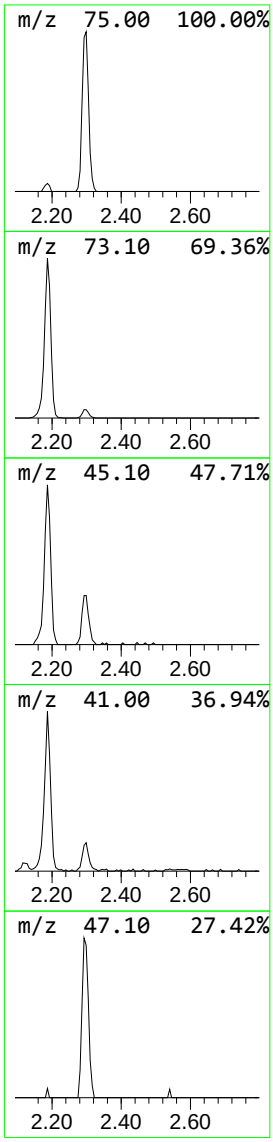
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.299	2.07 ng	46622	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
4	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7
5	Glycine	75	C2H5NO2	000056-40-6	7





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Data File : BF131131.D
Acq On : 10 Nov 2022 19:37
Operator : CG\JU
Sample : N5491-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

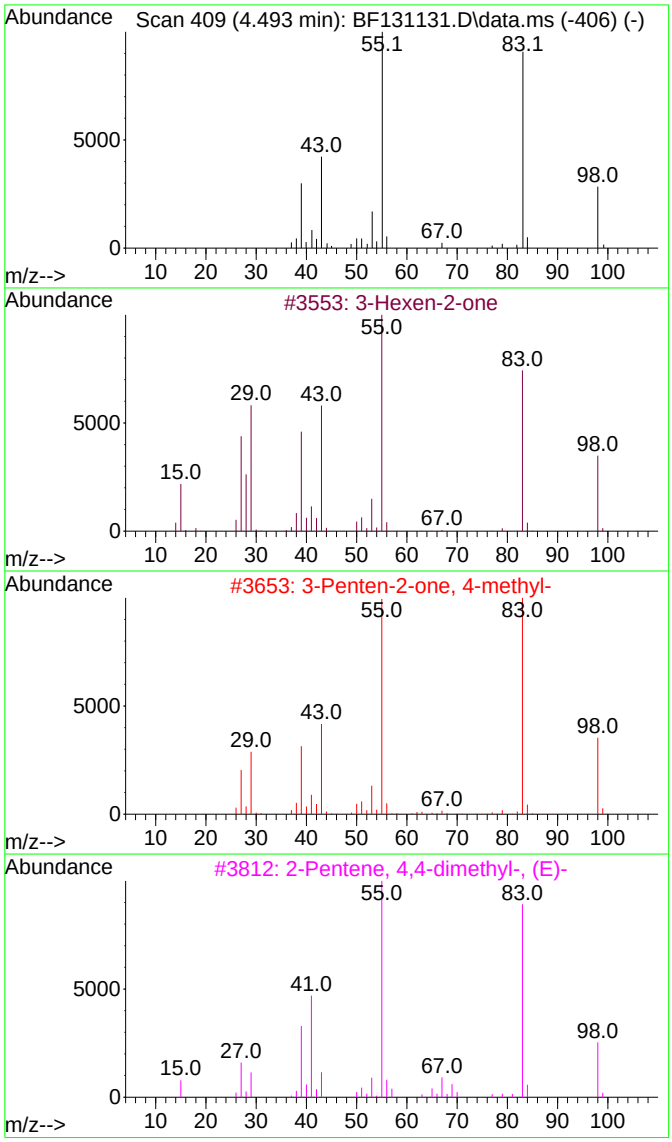
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

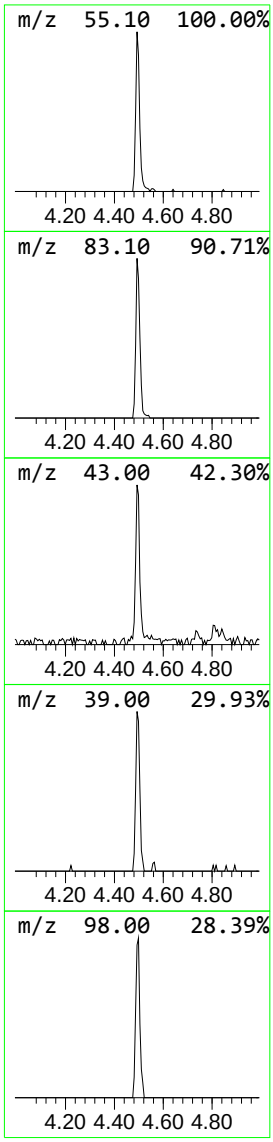
****

Peak Number 3 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.493	2.80 ng	63195	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78
4	2,4-Azetidinedione, 3,3-diethyl-	141	C7H11NO2	042282-85-9	78
5	Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	72





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Operator : CG\JU
Sample : N5491-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

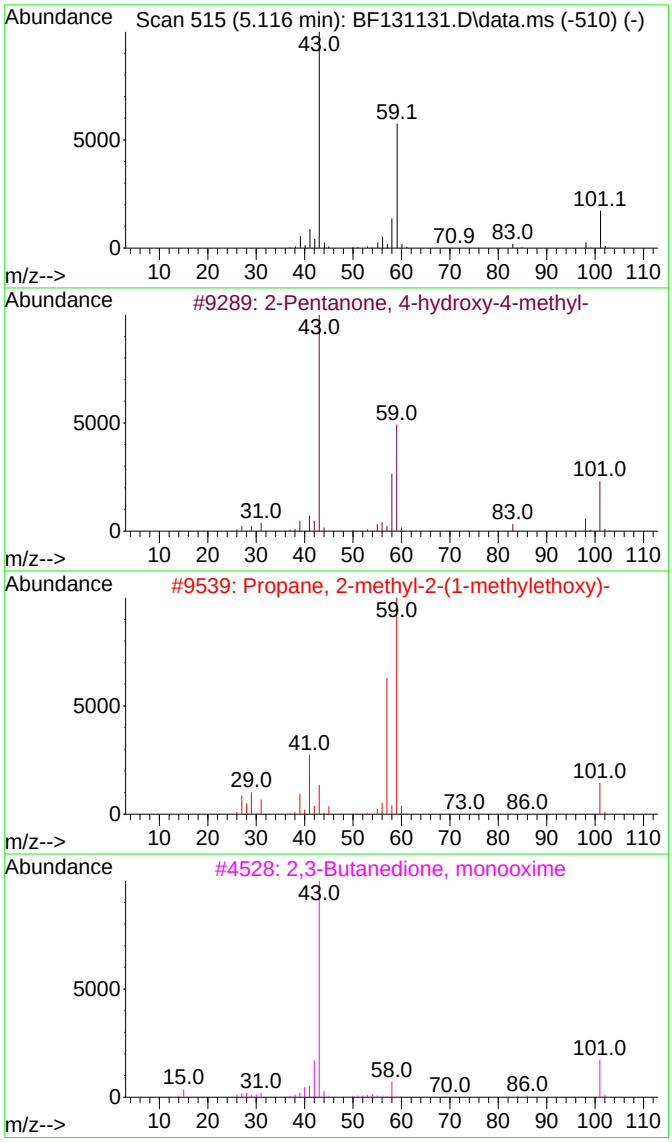
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

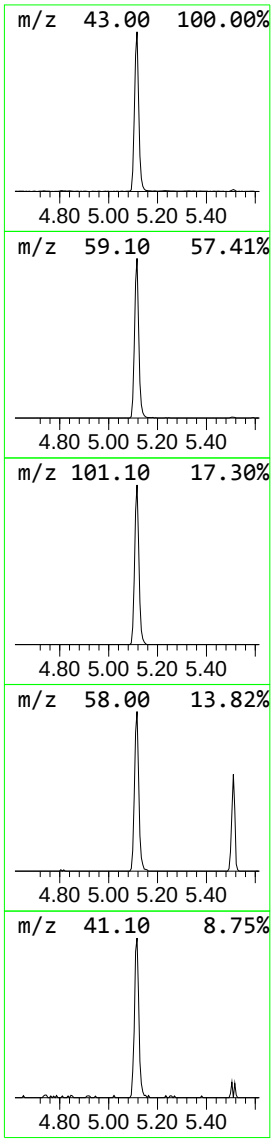
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	22.19 ng	500937	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131131.D
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Operator : CG\JU
Sample : N5491-01
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

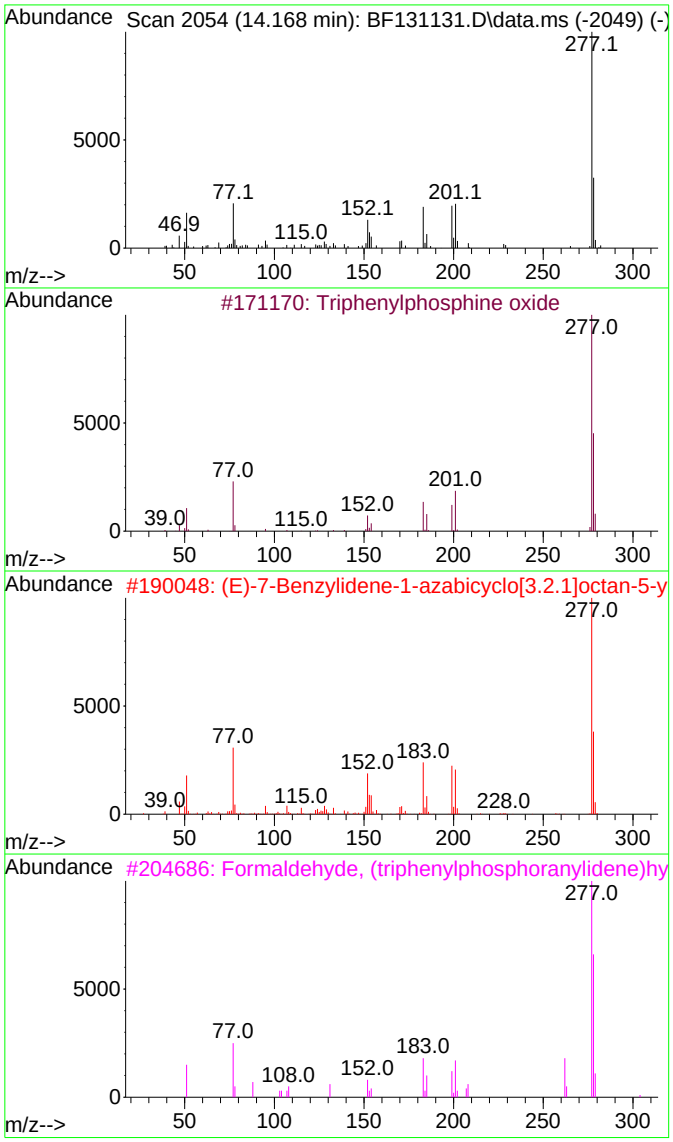
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

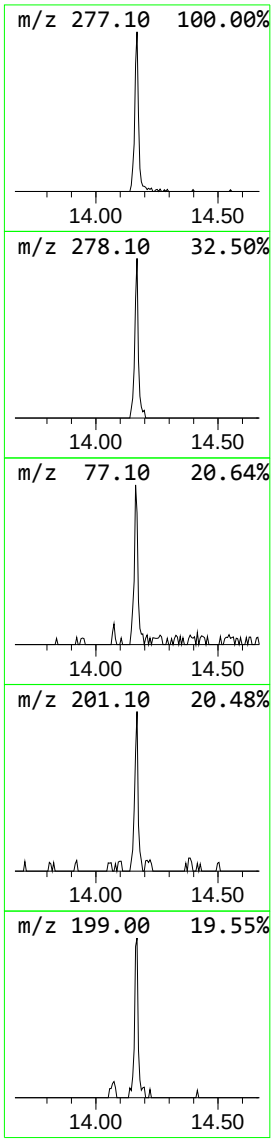
****

Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.169	3.18 ng	66220	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	86
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	68
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	43
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

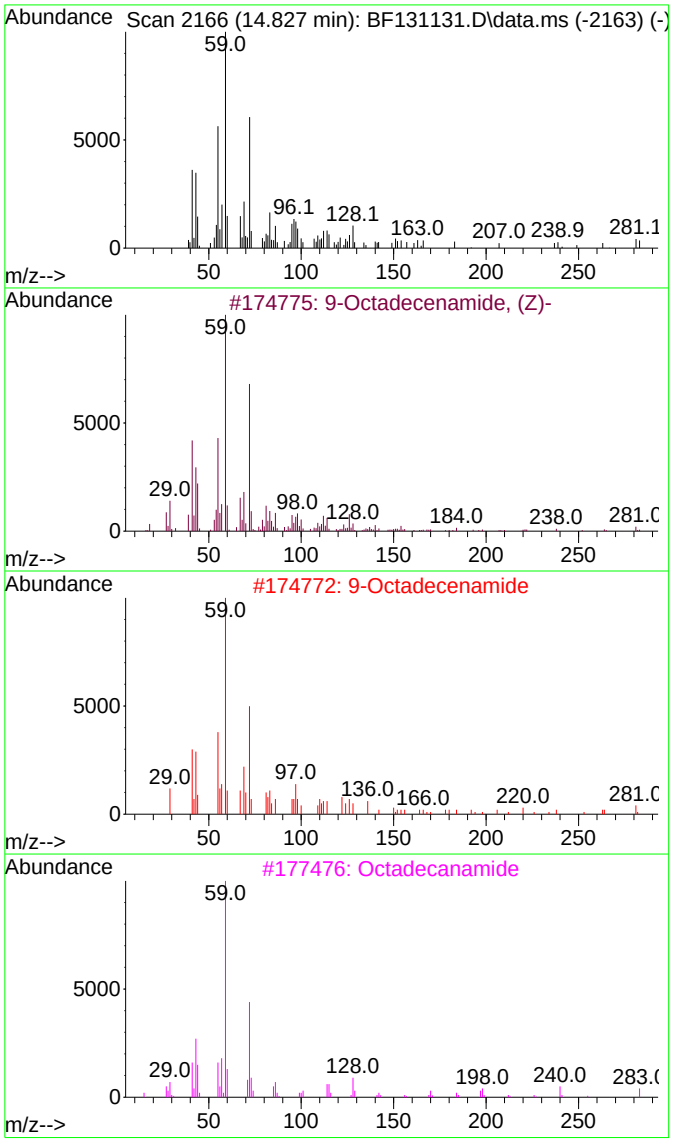
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

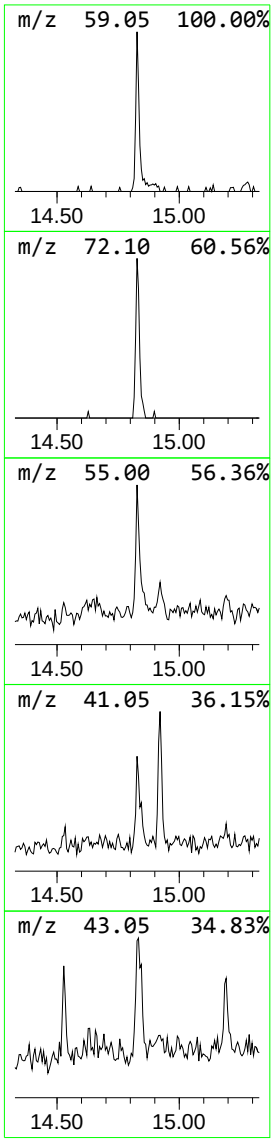
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.827	2.46 ng	57388	Perylene-d12	15.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2	9-Octadecenamide	281	C18H35NO	003322-62-1	76
3	Octadecanamide	283	C18H37NO	000124-26-5	64
4	Palmitoleamide	253	C16H31NO	106010-22-4	59
5	Hexadecanamide	255	C16H33NO	000629-54-9	59





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ClientSampleId :
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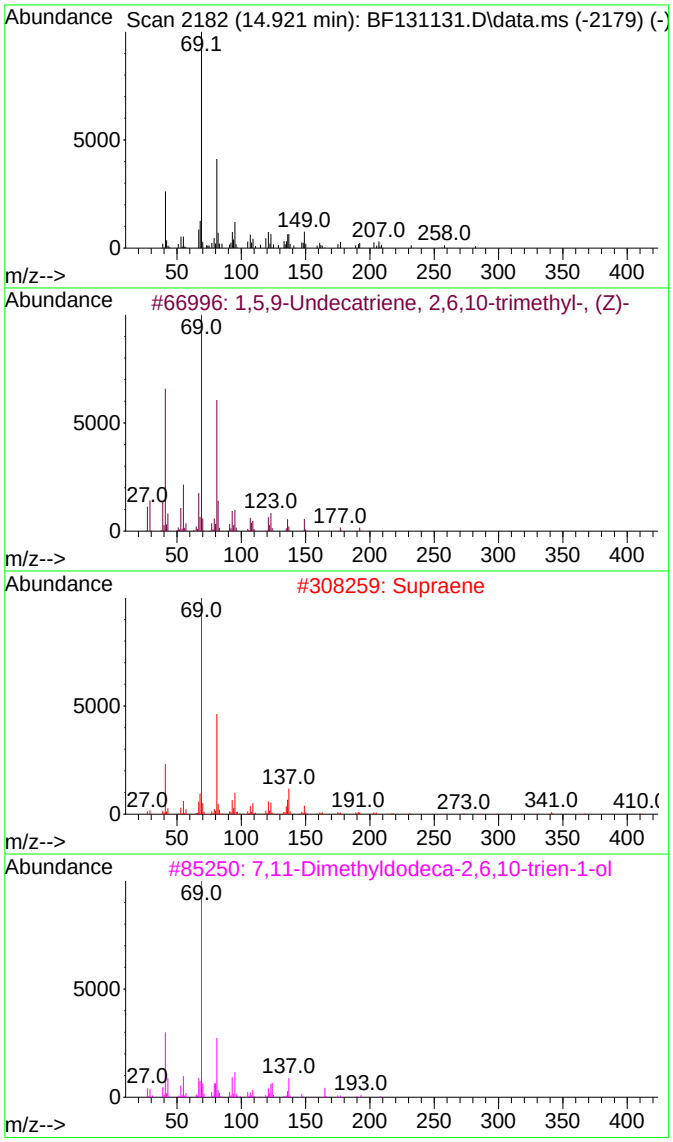
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

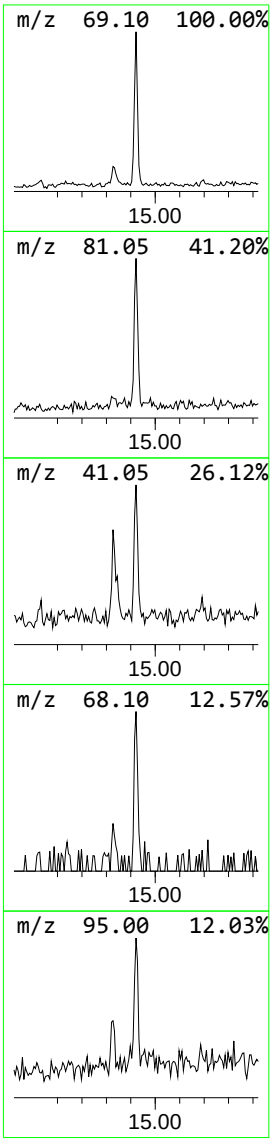
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	2.08 ng	48492	Perylene-d12	15.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	86
2	Supraene	410	C30H50	007683-64-9	80
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
4	(2E,6E)-3,7,11-Trimethyldodeca-2...	376	C25H44O2	078368-57-7	64
5	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.187	22.0	ng	496491	1	6.887	451482	20.0
Propane, 1,1-di...	2.299	2.1	ng	46622	1	6.887	451482	20.0
3-Hexen-2-one	4.493	2.8	ng	63195	1	6.887	451482	20.0
2-Pentanone, 4-...	5.116	22.2	ng	500937	1	6.887	451482	20.0
Triphenylphosph...	14.169	3.2	ng	66220	5	14.074	415833	20.0
9-Octadecenamid...	14.827	2.5	ng	57388	6	15.568	466963	20.0
1,5,9-Undecatri...	14.921	2.1	ng	48492	6	15.568	466963	20.0