LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131141.D
Acq On : 11 Nov 2022 00:45
Operator : CG\JU
Sample : N5491-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2

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: BF131141.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	19	rVB	421620	542891	39.34%	5.398%
2	2.246	22	27	38	rVB	26434	37269	2.70%	0.371%
3	4.481	403	407	412	rBV	42395	48475	3.51%	0.482%
4	5.104	509	513	524	rBV	319030	356747	25.85%	3.547%
5	5.504	577	581	596	rBV	1526703	1380103	100.00%	13.721%
6	6.516	748	753	756	rBV	1476413	1280276	92.77%	12.729%
7	6.887	813	816	820	rBV	497215	380364	27.56%	3.782%
8	7.451	908	912	915	rBV	949597	819035	59.35%	8.143%
9	8.175	1031	1035	1038	rBV	461260	418633	30.33%	4.162%
10	9.245	1213	1217	1221	rBV	1374417	1187073	86.01%	11.802%
11	9.934	1330	1334	1337	rBV	442922	384823	27.88%	3.826%
12	10.722	1464	1468	1478	rBV	836070	696608	50.48%	6.926%
13	11.422	1584	1587	1591	rBV	483265	409457	29.67%	4.071%
14	12.875	1831	1834	1836	rBV2	16738	18032	1.31%	0.179%
15	13.016	1853	1858	1861	rBV	1407544	1266335	91.76%	12.590%
16	13.574	1950	1953	1956	rBV4	16300	18870	1.37%	0.188%
17	13.904	2007	2009	2014	rBV2	23089	27716	2.01%	0.276%
18	14.074	2034	2038	2041	rBV	401328	379083	27.47%	3.769%
19	14.163	2051	2053	2059	rVB	50835	52884	3.83%	0.526%
20	14.533	2113	2116	2118	rBV2	26700	24487	1.77%	0.243%
21	14.827	2164	2166	2171	rBV4	34532	40828	2.96%	0.406%
22	15.568	2288	2292	2299	rVB2	194716	259829	18.83%	2.583%
23	17.809	2669	2673	2676	rBV6	21493	28371	2.06%	0.282%

Sum of corrected areas: 10058189

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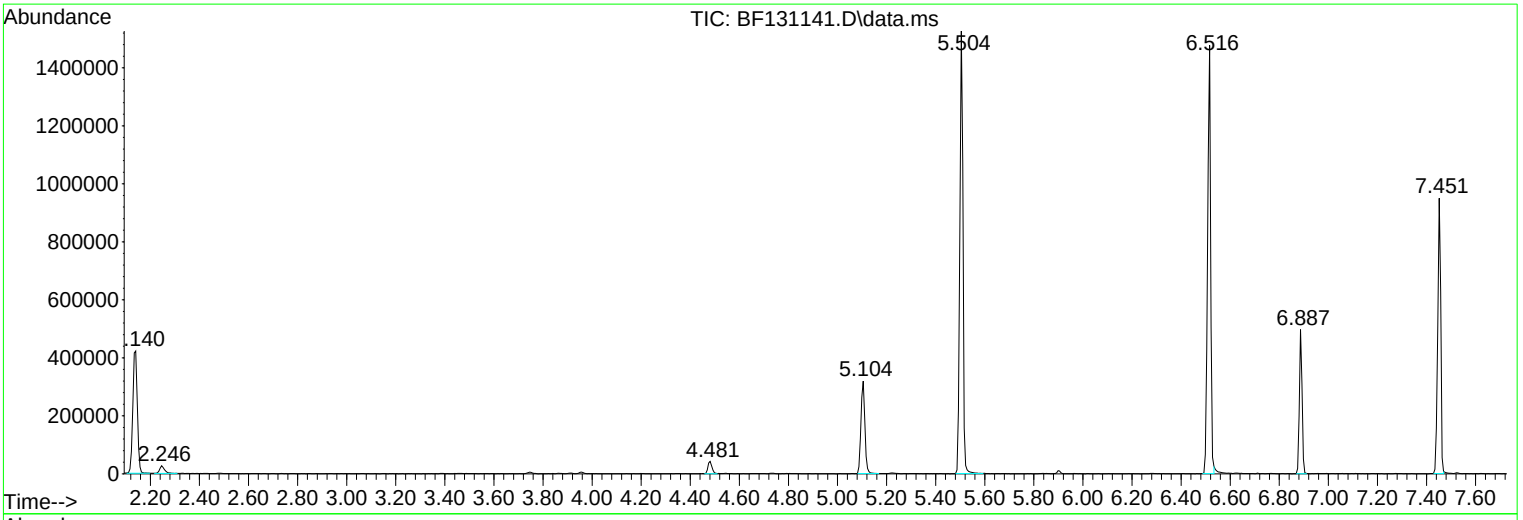
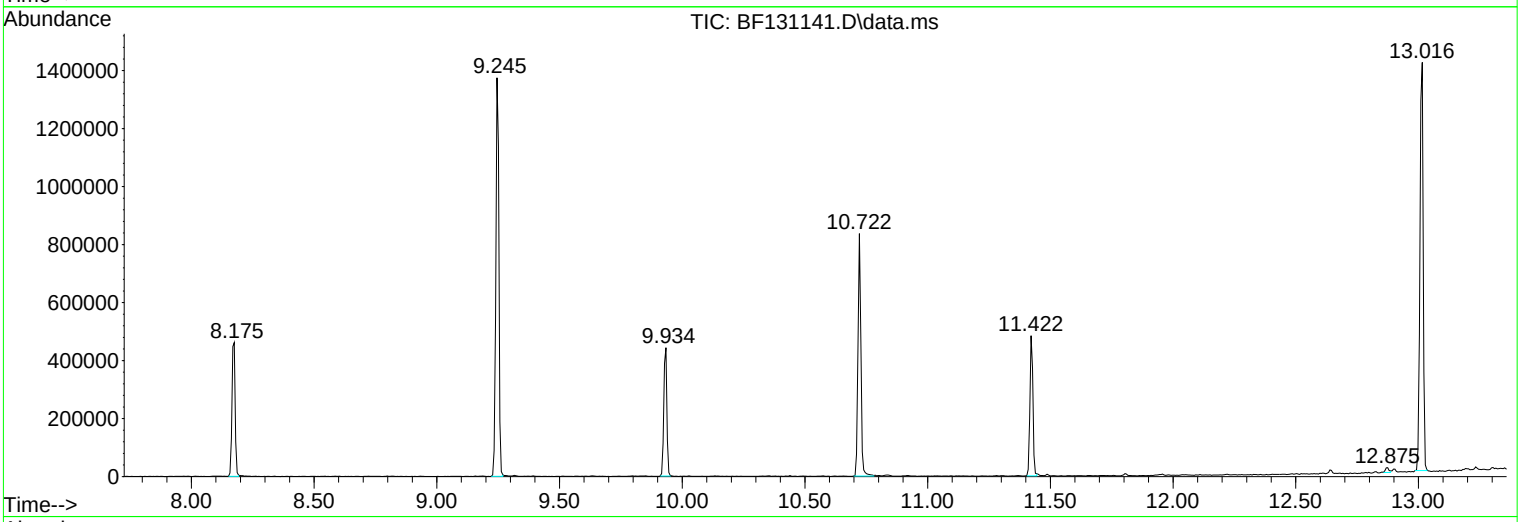
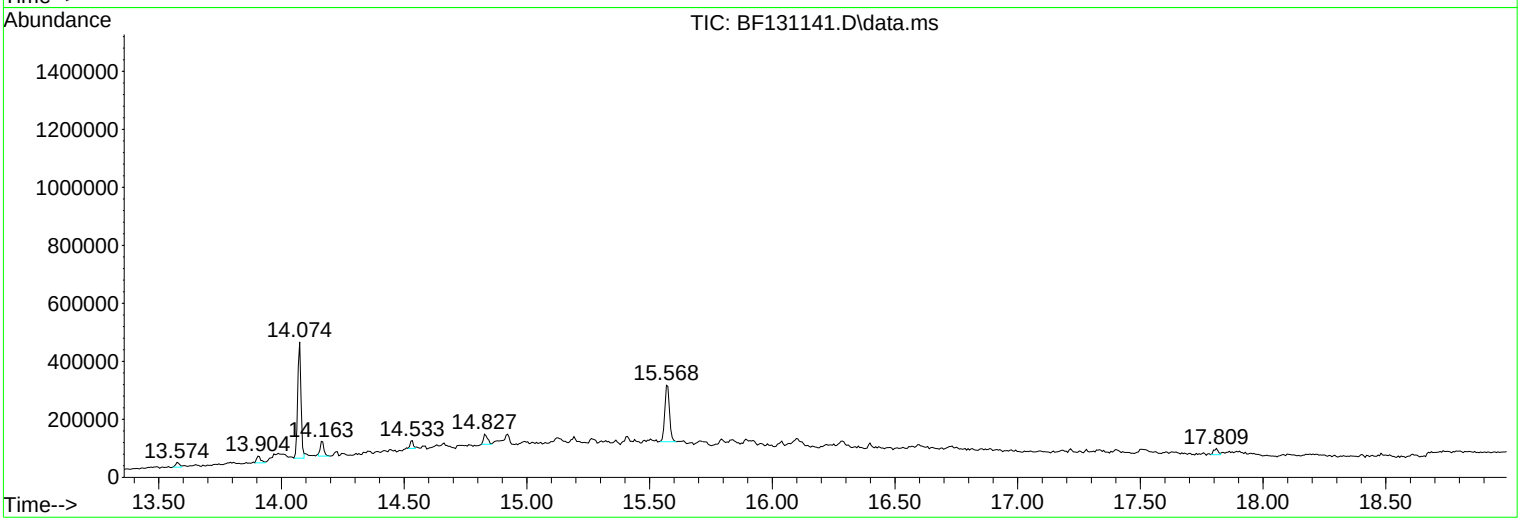
Instrument :
BNA_F
ClientSampleId :
TP-2

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

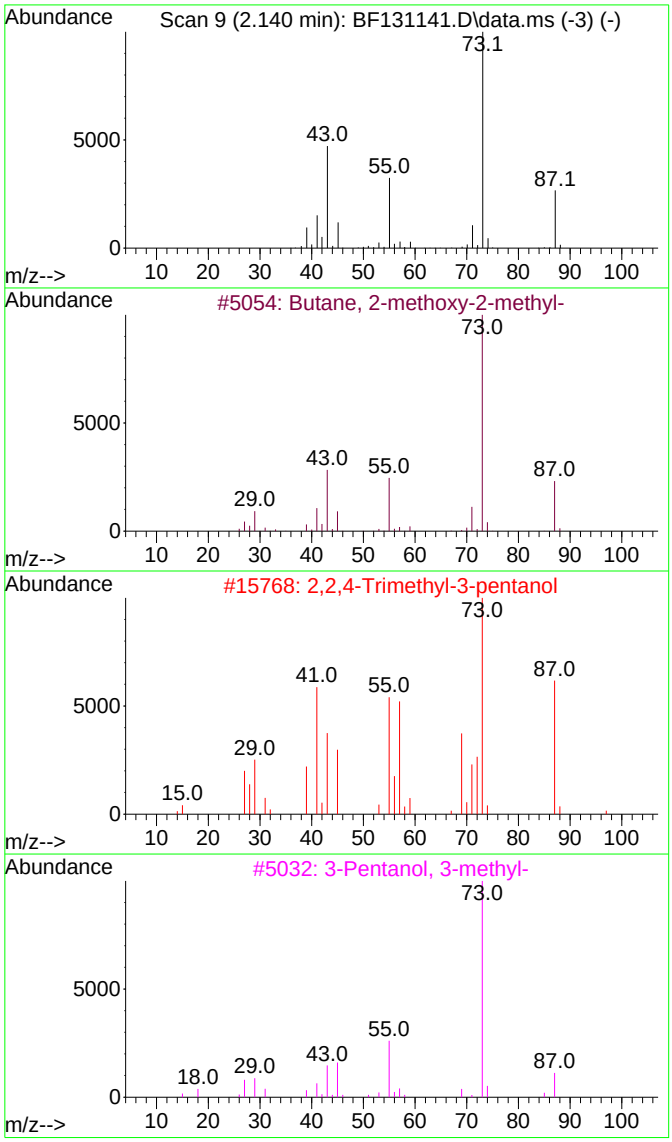
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

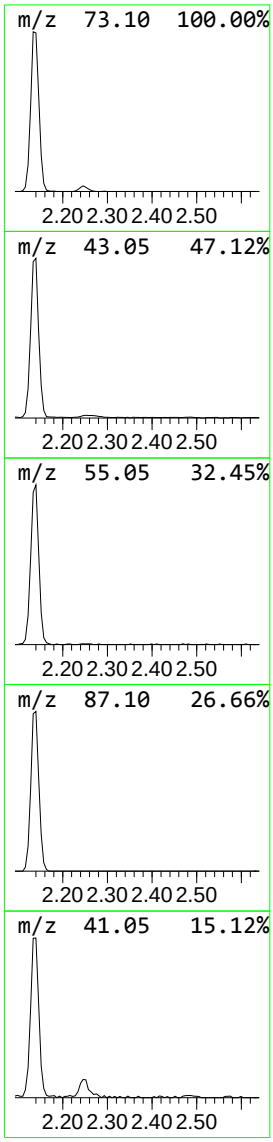
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	28.55 ng	542891	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	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Misc :
ALS Vial : 18 Sample Multiplier: 1

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
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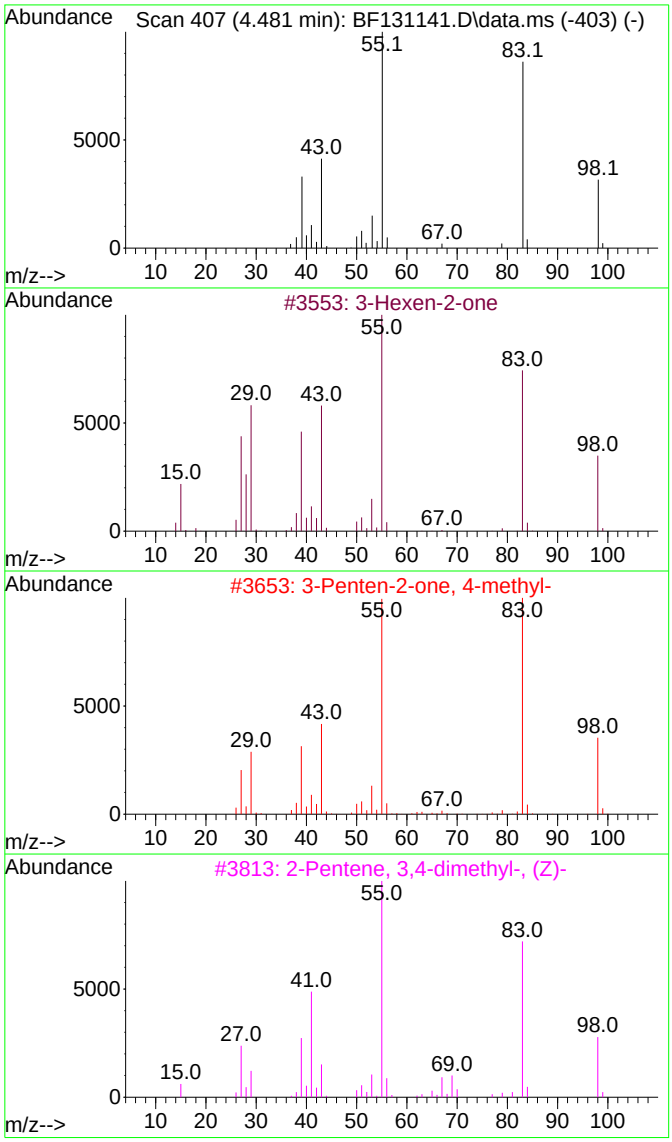
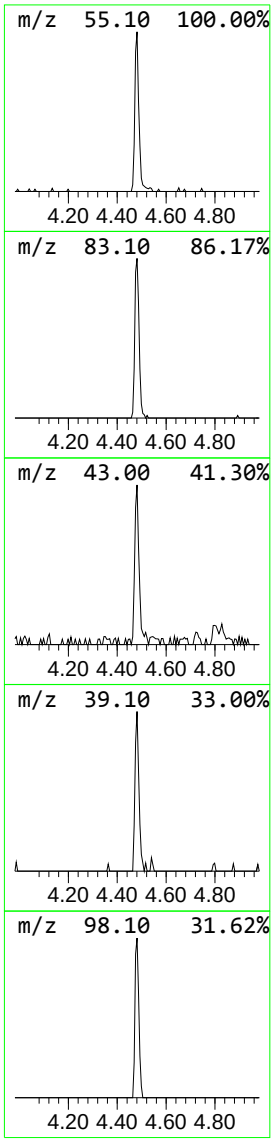
Peak Number 2 3-Hexen-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.481	2.55 ng	48475	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, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	64
5	Cyclohexane, methyl-	98	C7H14	000108-87-2	59





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Acq On : 11 Nov 2022 00:45
Operator : CG\JU
Sample : N5491-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

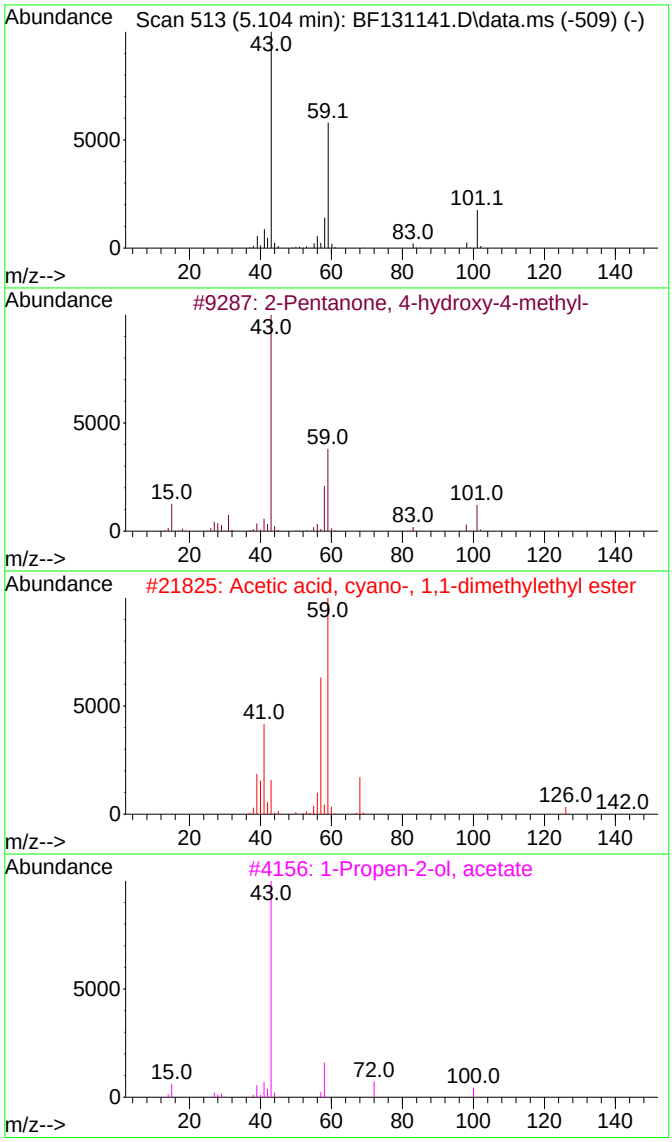
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

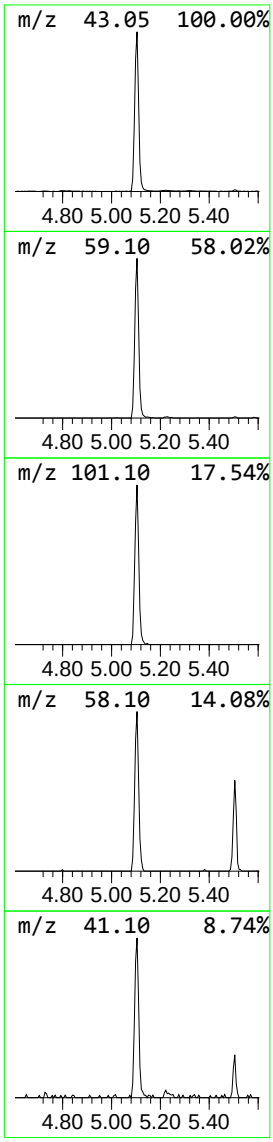
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	18.76 ng	356747	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	42
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





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Sample : N5491-04
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
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TIC Library : C:\Database\NIST20.L
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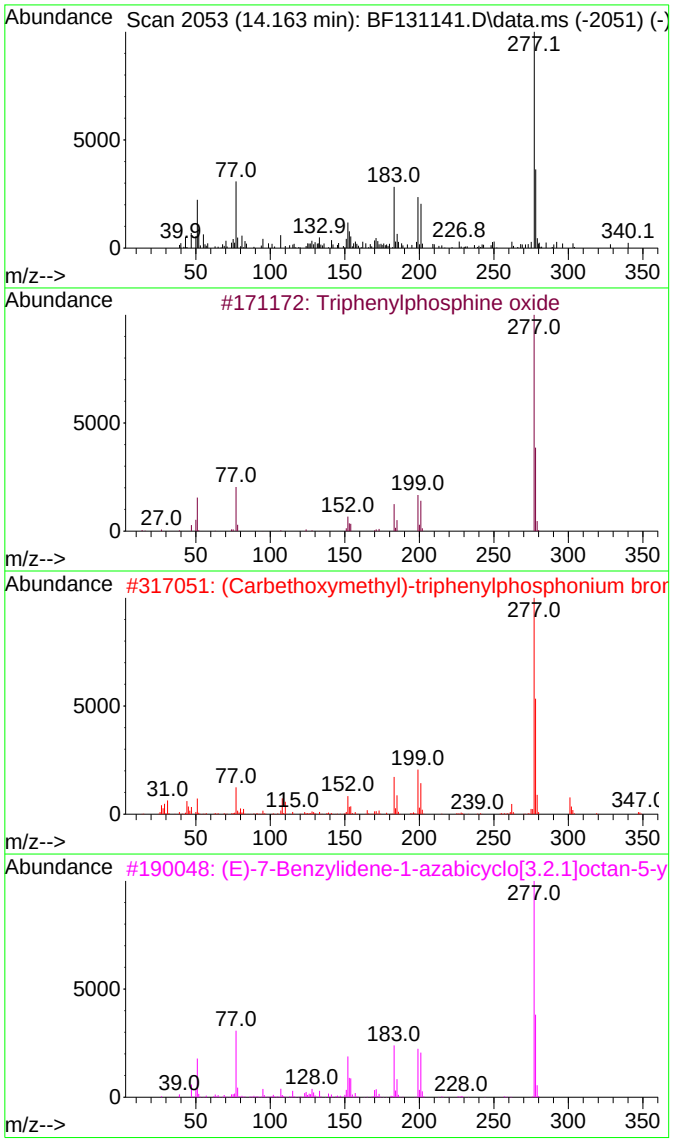
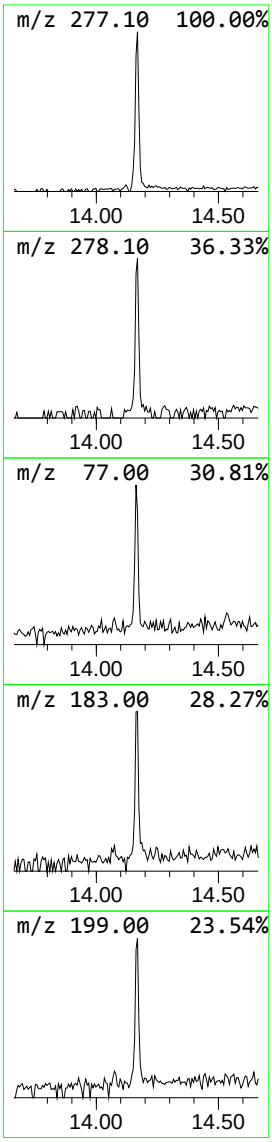
Peak Number 4 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.163	2.79 ng	52884	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	43
3	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	43
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	38
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	37





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Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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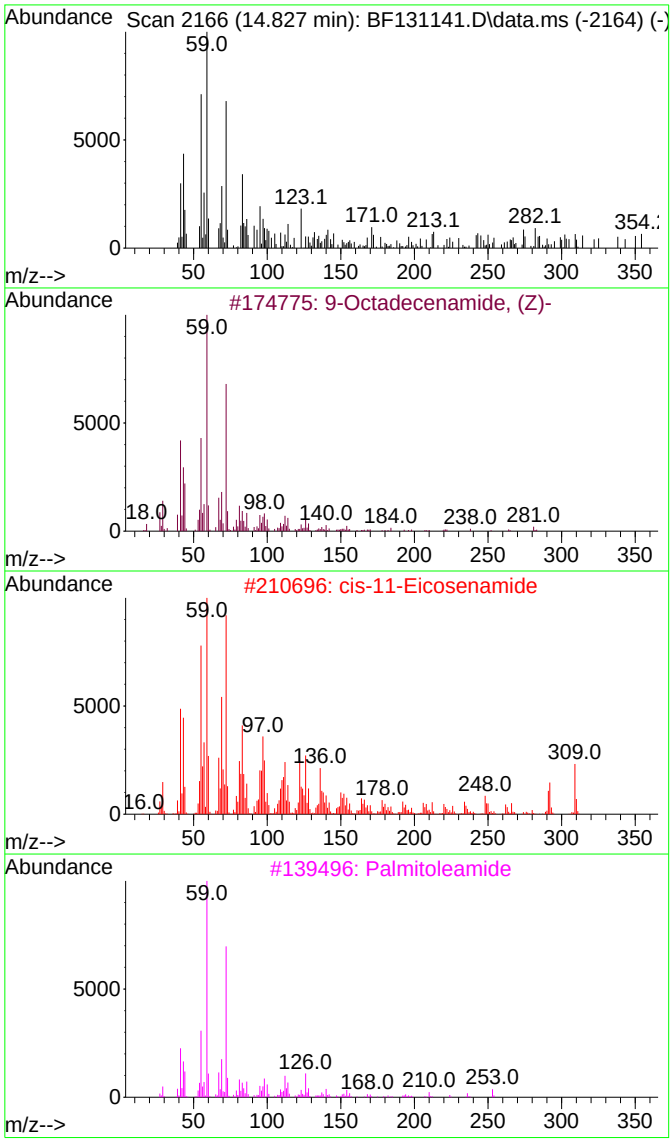
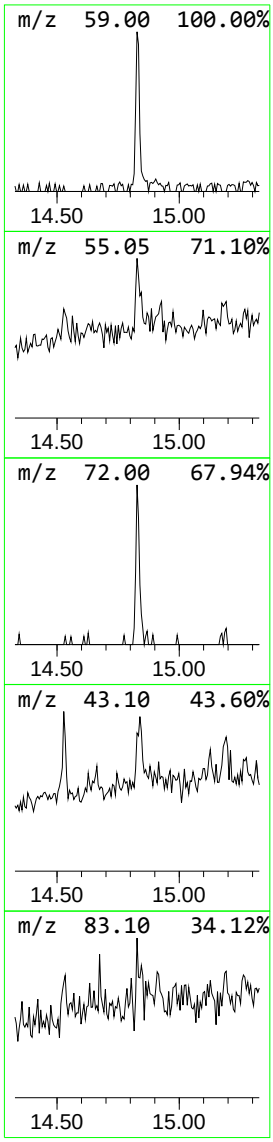
Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.827	3.14 ng	40828	Perylene-d12	15.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2	cis-11-Eicosenamide	309	C20H39NO	010436-08-5	58
3	Palmitoleamide	253	C16H31NO	106010-22-4	53
4	Dodecanamide	199	C12H25NO	001120-16-7	46
5	Octanamide	143	C8H17NO	000629-01-6	43





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Instrument :
BNA_F
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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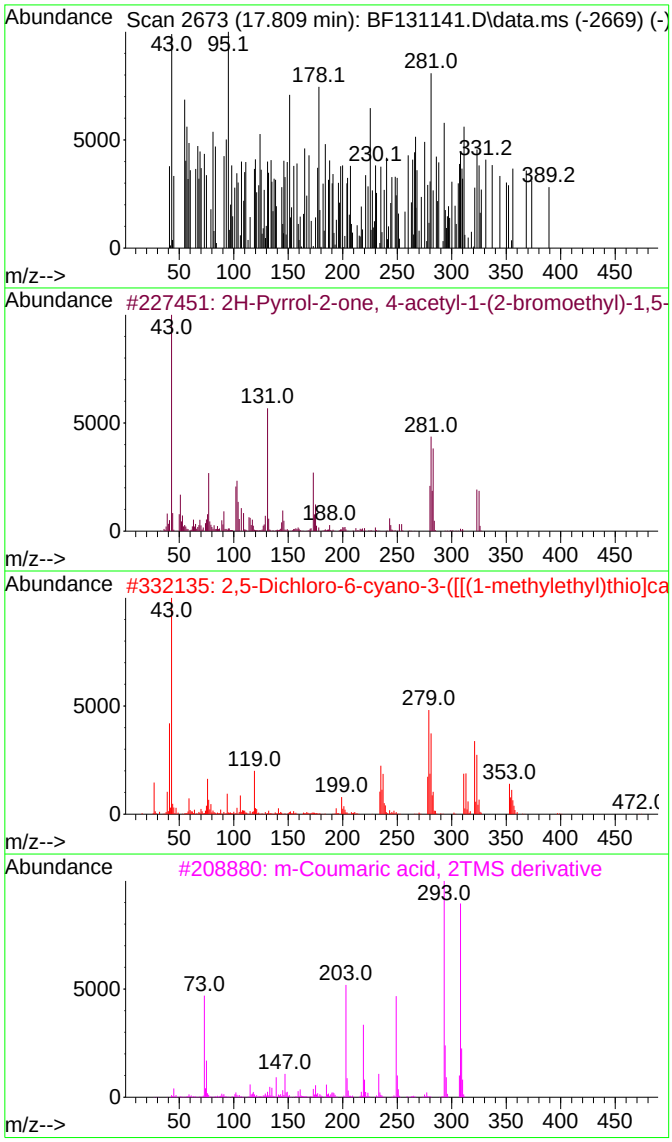
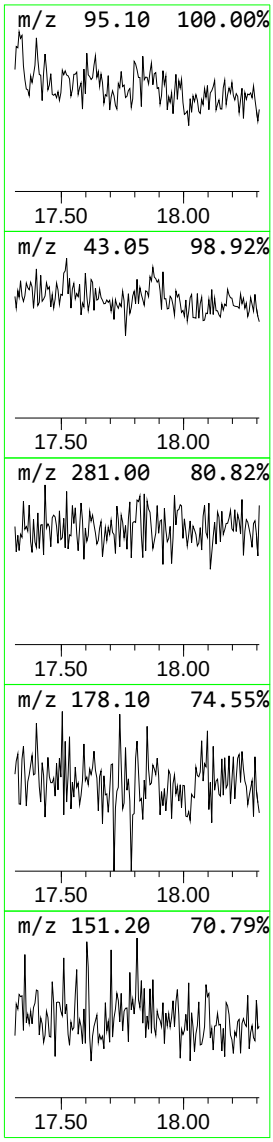
Peak Number 6 unknown17.810 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.810	2.18 ng	28371	Perylene-d12	15.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyrrol-2-one, 4-acetyl-1-(2-b...	323	C14H14BrNO3	1000350-70-5	30
2	2,5-Dichloro-6-cyano-3-([[(1-met...	472	C14H14Cl2N2S6	1000305-32-5	12
3	m-Coumaric acid, 2TMS derivative	308	C15H24O3Si2	032342-01-1	11
4	Acetamide, N-(5-bromo2-cycloprop...	321	C14H12BrNO3	309267-08-1	10
5	2,4-Di-tert-butyl-6-(1-hydroxy-1...	326	C22H30O2	1000388-38-8	10





Tentatively Identified Compound (LSC) summary

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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...	2.140	28.6	ng	542891	1	6.887	380364	20.0
3-Hexen-2-one	4.481	2.5	ng	48475	1	6.887	380364	20.0
2-Pentanone, 4-...	5.104	18.8	ng	356747	1	6.887	380364	20.0
Triphenylphosph...	14.163	2.8	ng	52884	5	14.074	379083	20.0
9-Octadecenamid...	14.827	3.1	ng	40828	6	15.568	259829	20.0
unknown17.810	17.810	2.2	ng	28371	6	15.568	259829	20.0