LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131142.D
Acq On : 11 Nov 2022 01:16
Operator : CG\JU
Sample : N5491-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

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: BF131142.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	4	10	16	rBV	440506	530704	43.80%	5.923%
2	2.257	22	29	36	rVB	25366	35770	2.95%	0.399%
3	4.481	403	407	414	rBV	38938	43919	3.62%	0.490%
4	5.104	509	513	523	rVB	280994	302453	24.96%	3.375%
5	5.504	577	581	585	rBV	1300794	1211644	100.00%	13.522%
6	6.516	749	753	756	rBV	1306922	1126176	92.95%	12.568%
7	6.887	813	816	820	rBV	422835	346175	28.57%	3.863%
8	7.451	908	912	915	rBV	816618	682408	56.32%	7.616%
9	8.175	1031	1035	1038	rBV	413835	349737	28.86%	3.903%
10	9.245	1214	1217	1221	rBV	1130472	1005000	82.95%	11.216%
11	9.933	1330	1334	1337	rBV	388626	326820	26.97%	3.647%
12	10.722	1464	1468	1478	rBV	689904	590819	48.76%	6.593%
13	11.422	1584	1587	1591	rBV	384549	351671	29.02%	3.925%
14	12.874	1828	1834	1836	rBV3	10435	13210	1.09%	0.147%
15	13.016	1853	1858	1861	rBV	1189762	1092860	90.20%	12.196%
16	13.233	1892	1895	1899	rBV3	12057	13638	1.13%	0.152%
17	13.574	1950	1953	1956	rBV2	19668	20184	1.67%	0.225%
18	13.910	2007	2010	2012	rVB	17768	17229	1.42%	0.192%
19	14.074	2034	2038	2044	rVB	436865	389761	32.17%	4.350%
20	14.168	2050	2054	2057	rBV	50607	54850	4.53%	0.612%
21	14.527	2113	2115	2118	rVB3	33424	28629	2.36%	0.319%
22	14.827	2163	2166	2175	rVB3	49662	88190	7.28%	0.984%
23	14.921	2179	2182	2187	rVB	49853	51712	4.27%	0.577%
24	15.574	2288	2293	2298	rBV	187439	255900	21.12%	2.856%
25	16.557	2457	2460	2463	rBV5	21730	31242	2.58%	0.349%

Sum of corrected areas: 8960701

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
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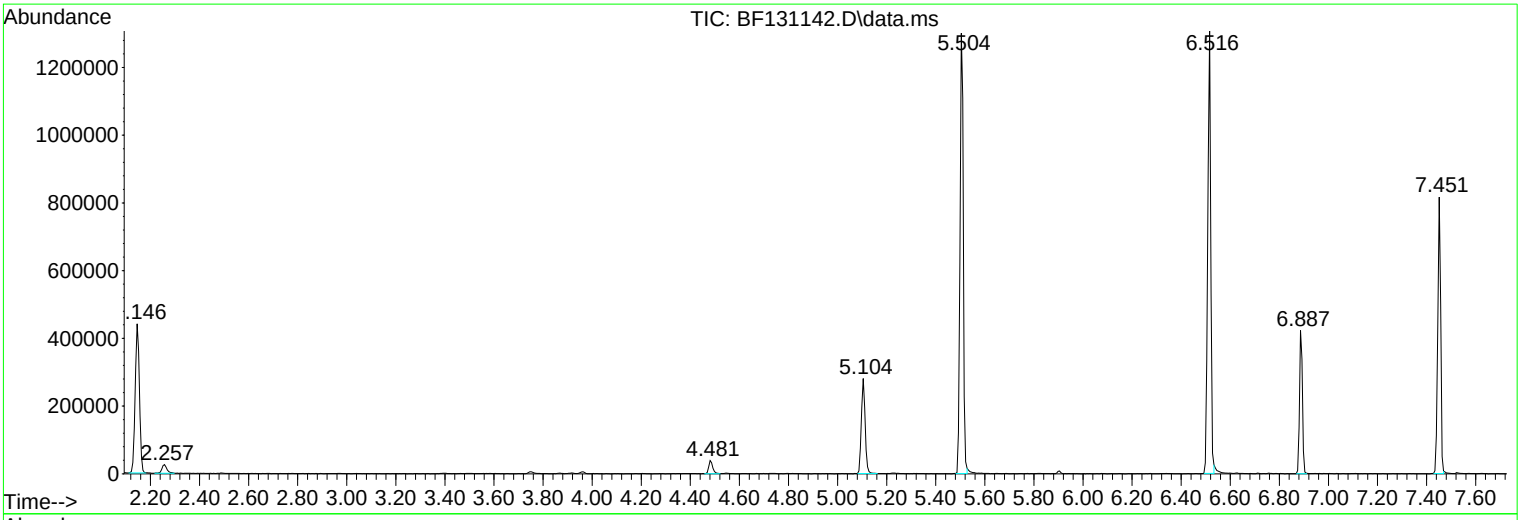
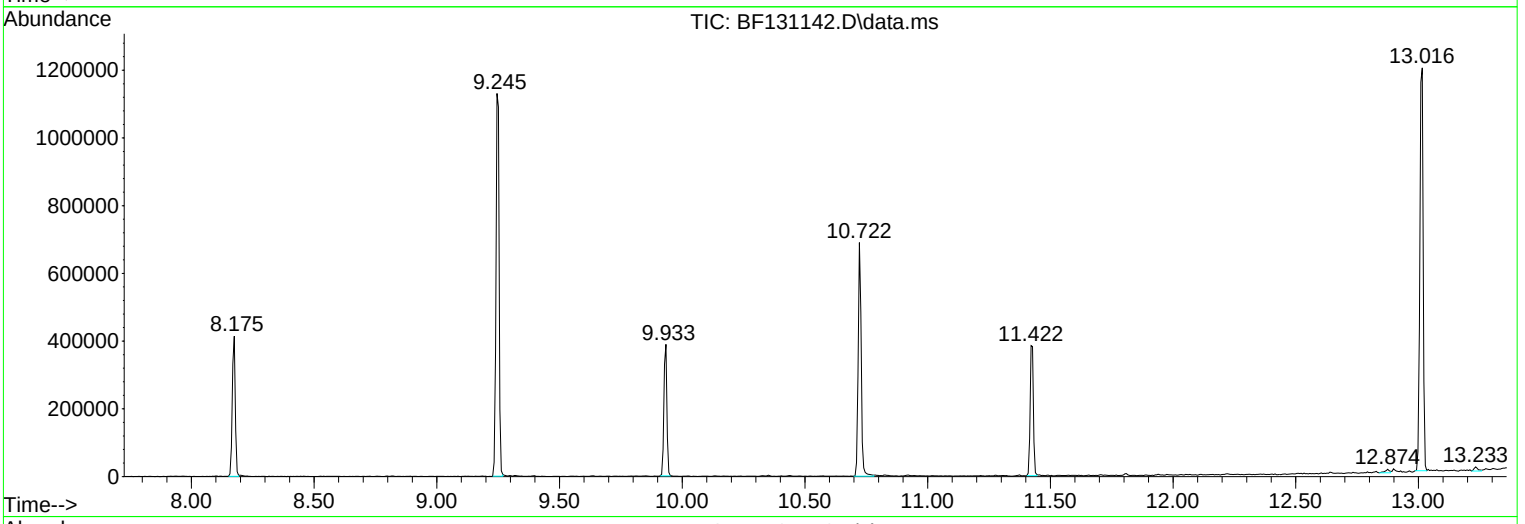
Sample : N5491-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

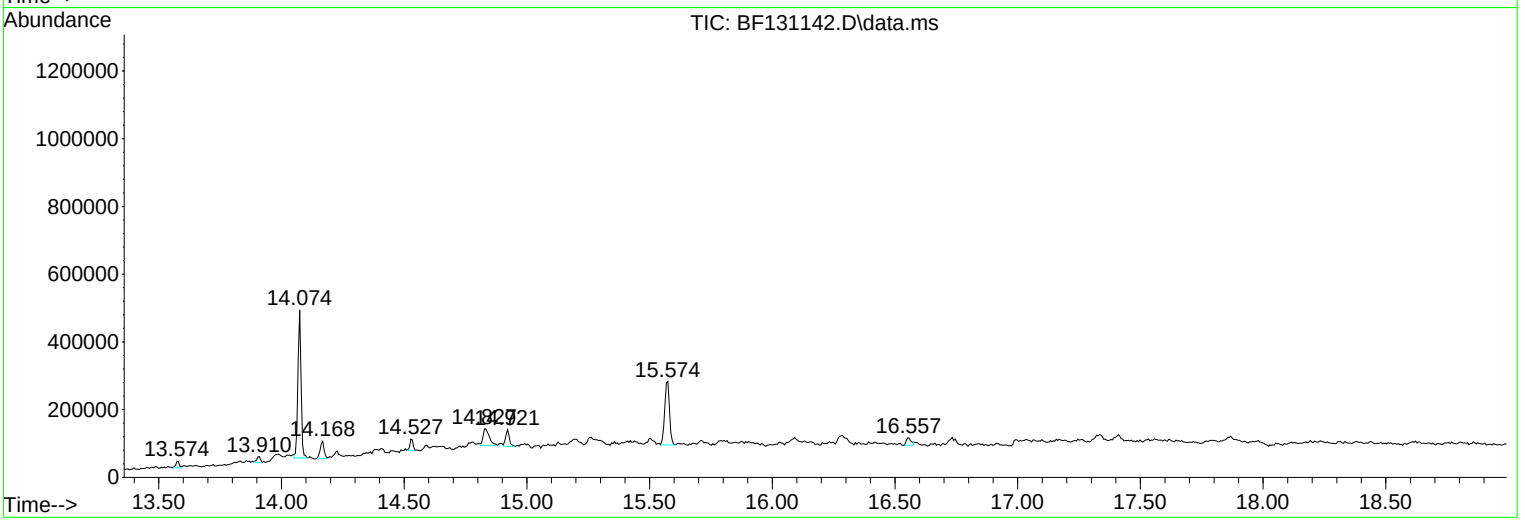
Instrument :
BNA_F
ClientSampleId :
TP-3

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131142.D
Acq On : 11 Nov 2022 01:16
Operator : CG\JU
Sample : N5491-07
Misc :
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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

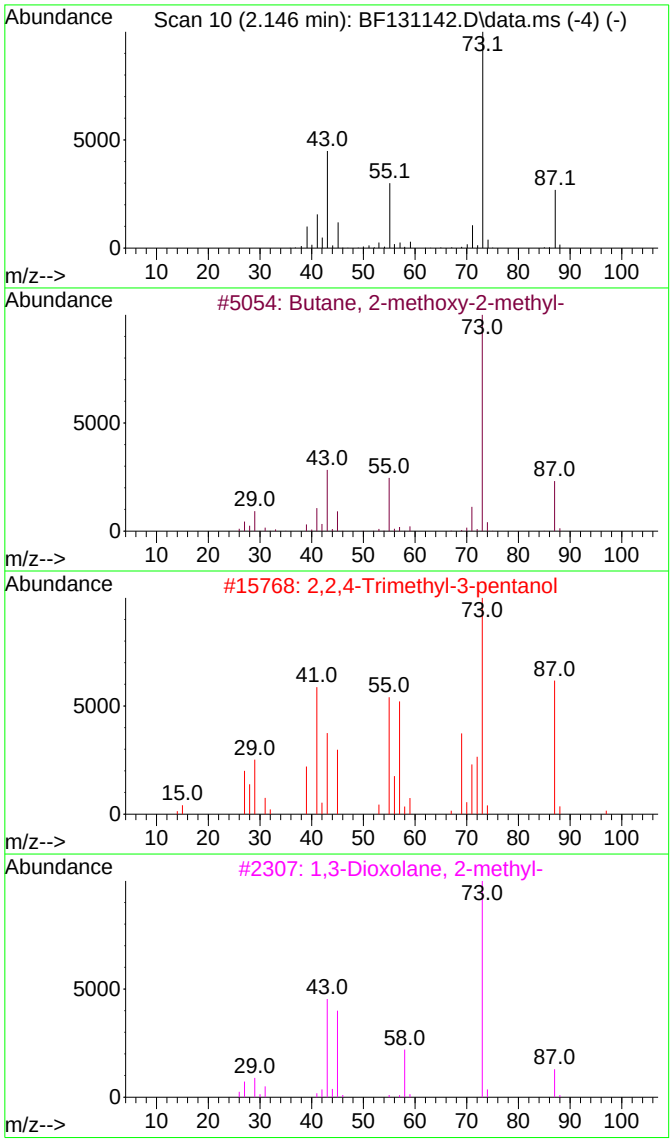
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

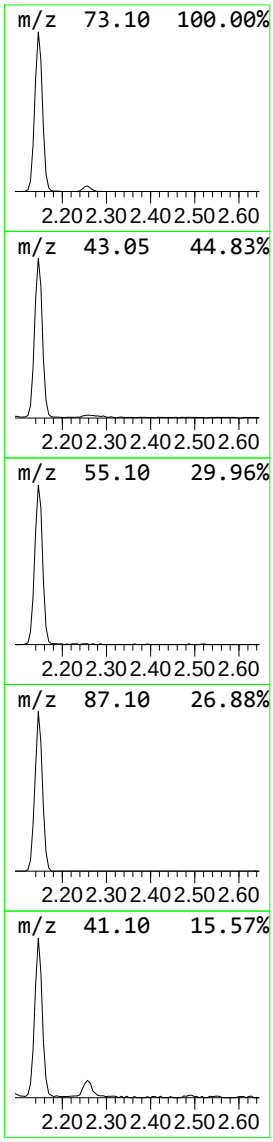
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	30.66 ng	530704	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	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131142.D
Acq On : 11 Nov 2022 01:16
Operator : CG\JU
Sample : N5491-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

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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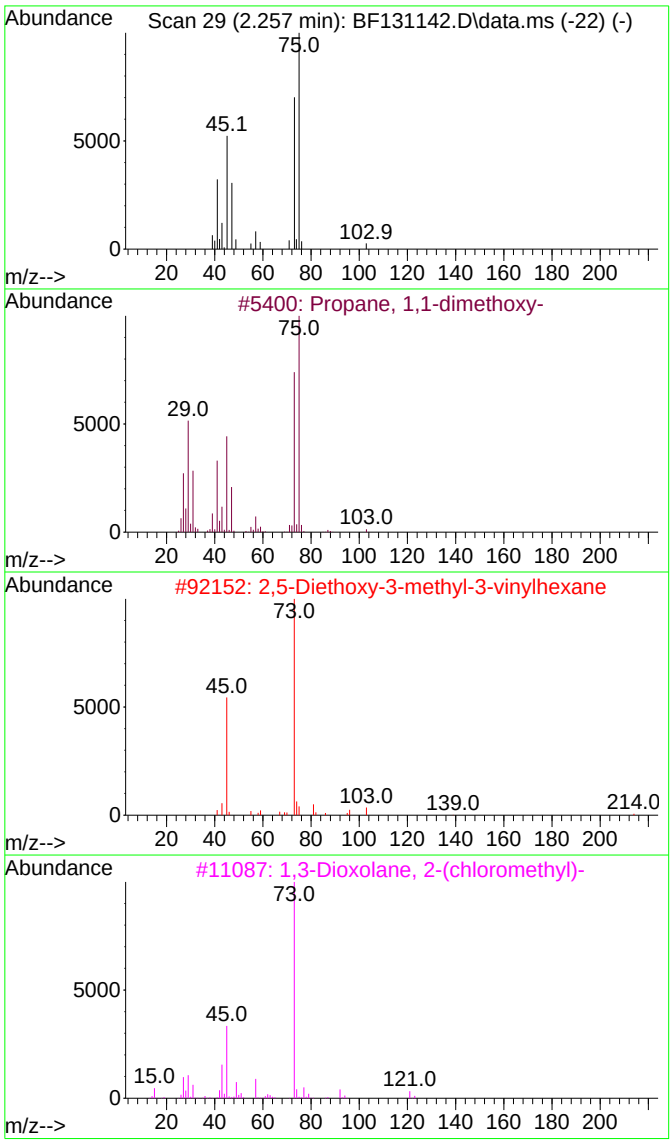
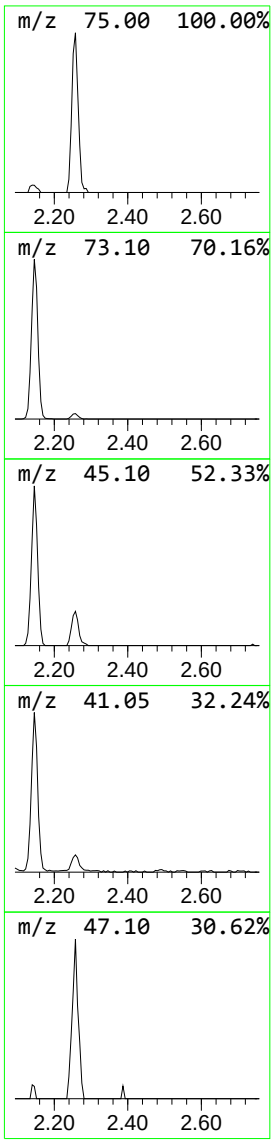
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	2.07 ng	35770	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	78
2	2,5-Diethoxy-3-methyl-3-vinylhexane	214	C13H26O2	1000432-70-8	10
3	1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
4	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
5	Disilane, pentamethyl(pentafluor...	298	C11H15F5Si2	033558-55-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131142.D
Acq On : 11 Nov 2022 01:16
Operator : CG\JU
Sample : N5491-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

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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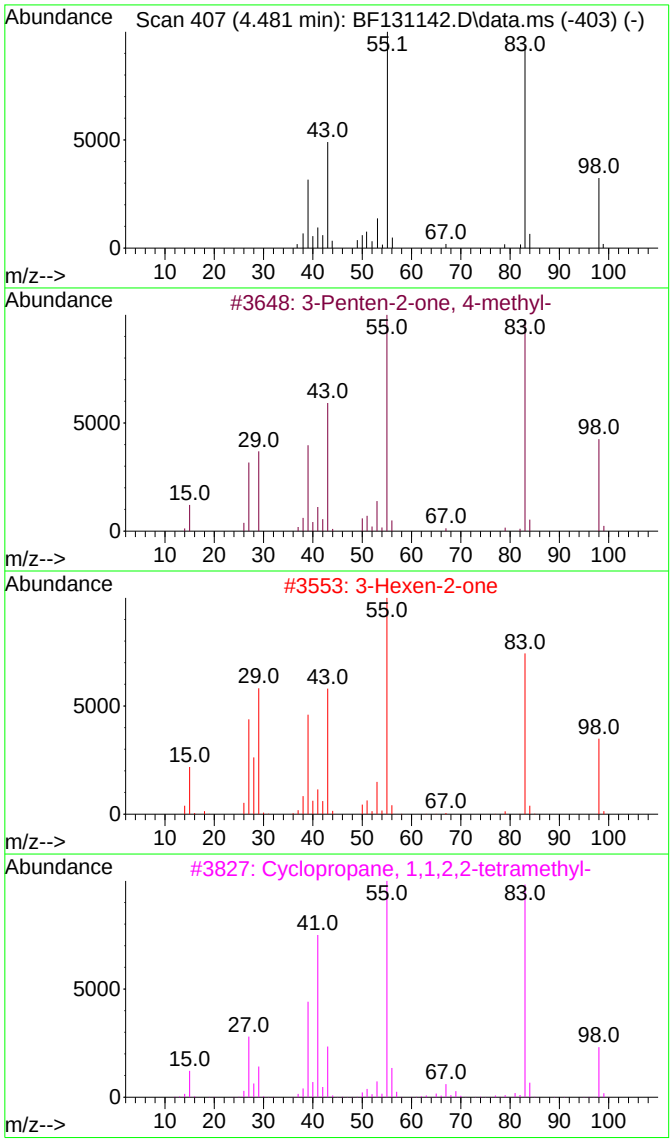
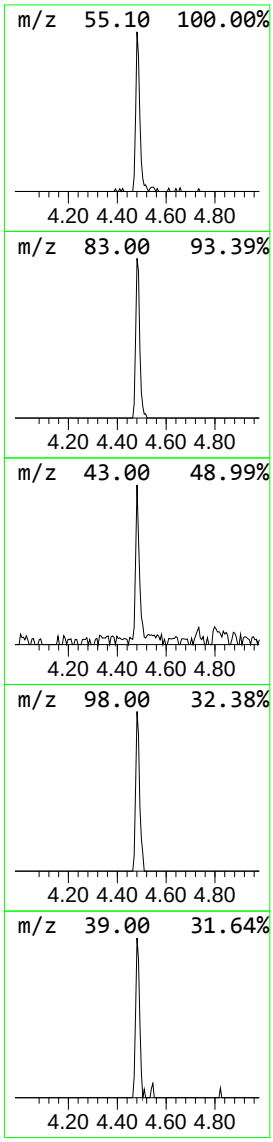
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.481	2.54 ng	43919	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	86
4	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	86
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131142.D
Acq On : 11 Nov 2022 01:16
Operator : CG\JU
Sample : N5491-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

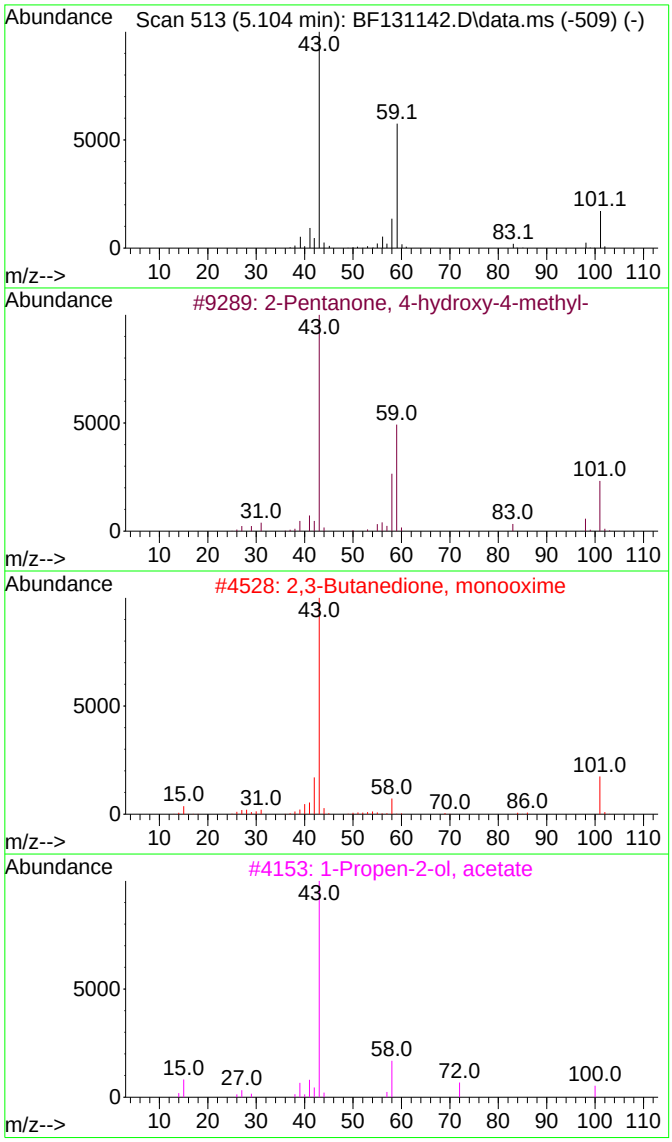
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

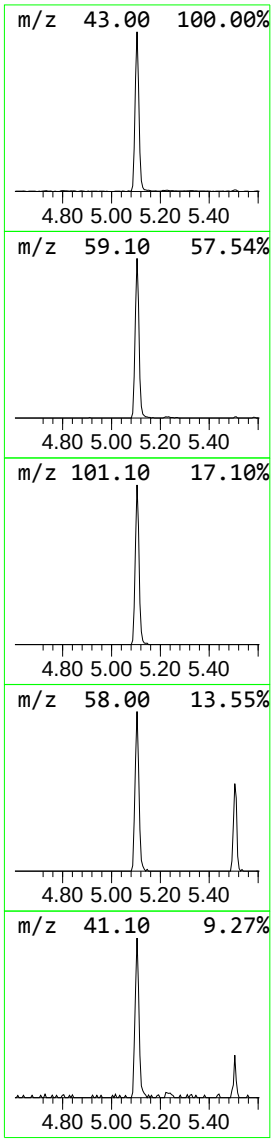
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	17.47 ng	302453	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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131142.D
Acq On : 11 Nov 2022 01:16
Operator : CG\JU
Sample : N5491-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

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

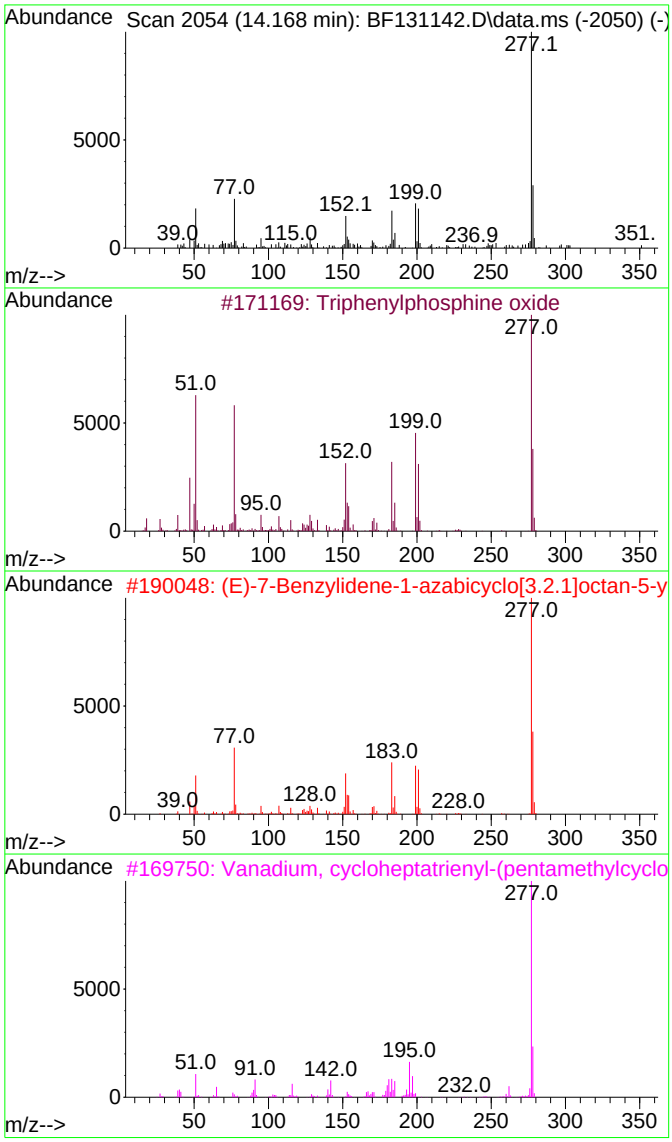
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

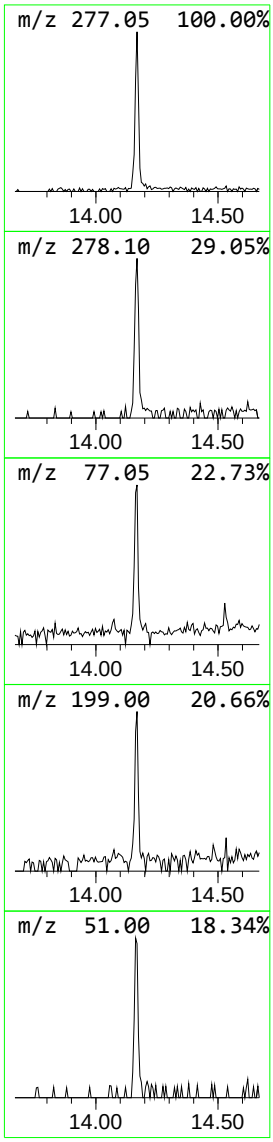
****

Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.169	2.81 ng	54850	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	50
4	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	47
5	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131142.D
Acq On : 11 Nov 2022 01:16
Operator : CG\JU
Sample : N5491-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

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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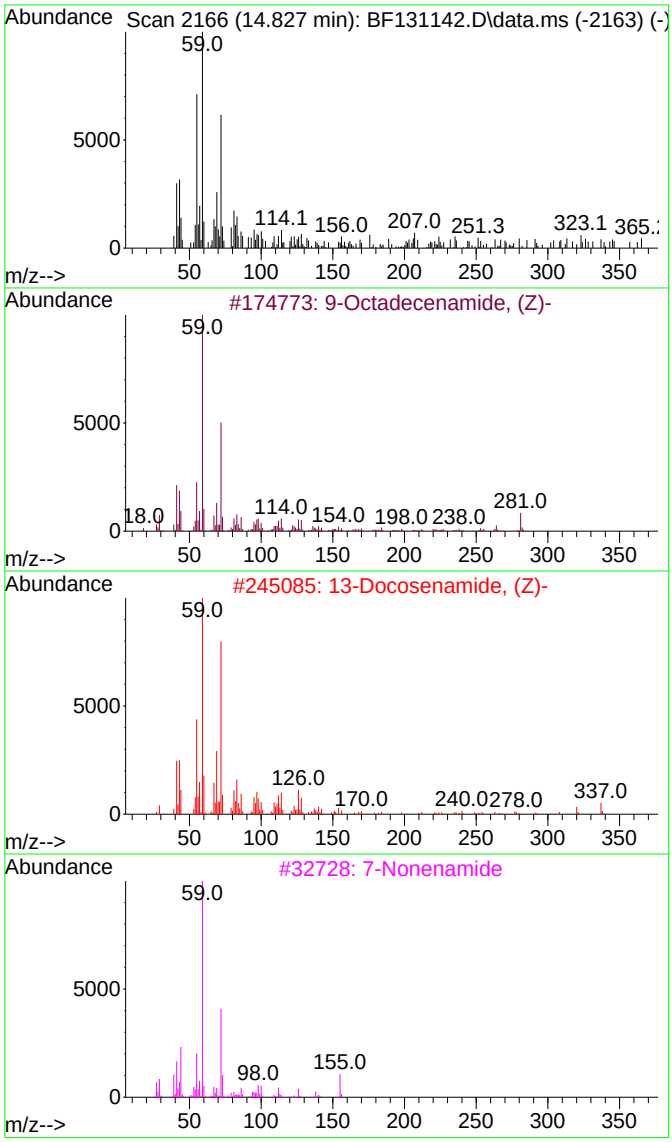
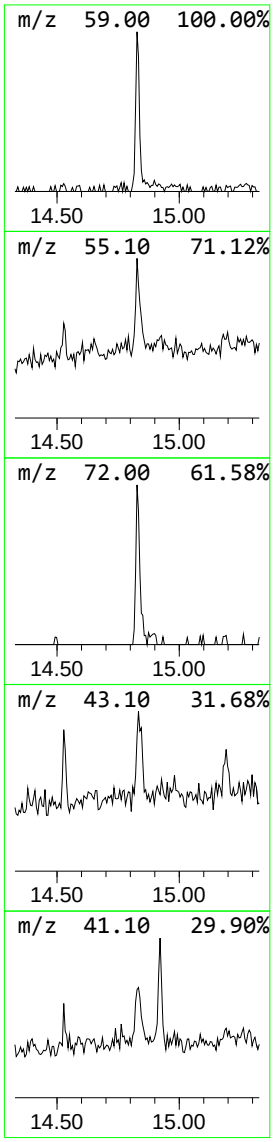
Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.827	6.89 ng	88190	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	68
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	50
3	7-Nonenamide	155	C9H17NO	090949-53-4	49
4	Tetradecanamide	227	C14H29NO	000638-58-4	49
5	Octadecanamide	283	C18H37NO	000124-26-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131142.D
Acq On : 11 Nov 2022 01:16
Operator : CG\JU
Sample : N5491-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

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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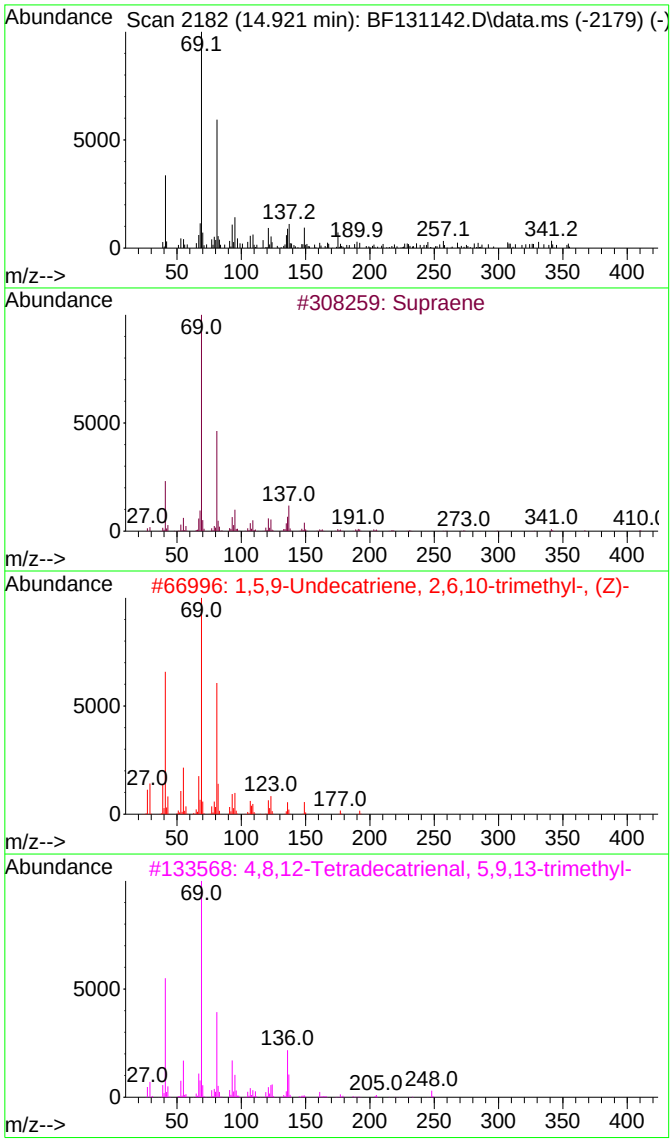
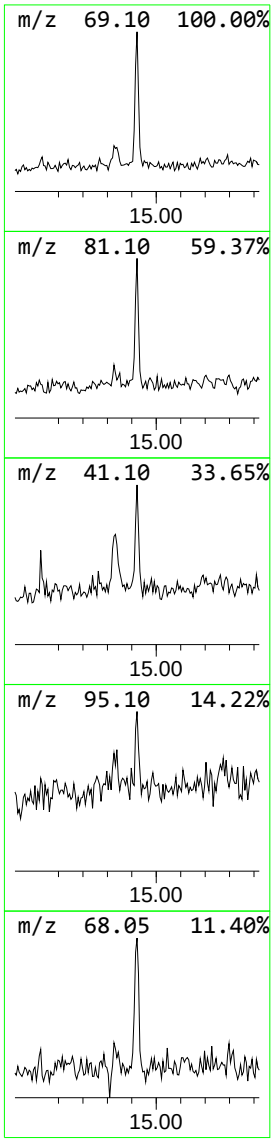
Peak Number 7 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	4.04 ng	51712	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	83
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	59
5	.beta.-Citronellol, chlorodifluo...	268	C12H19ClF2O2	1000376-20-8	52





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Sample : N5491-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

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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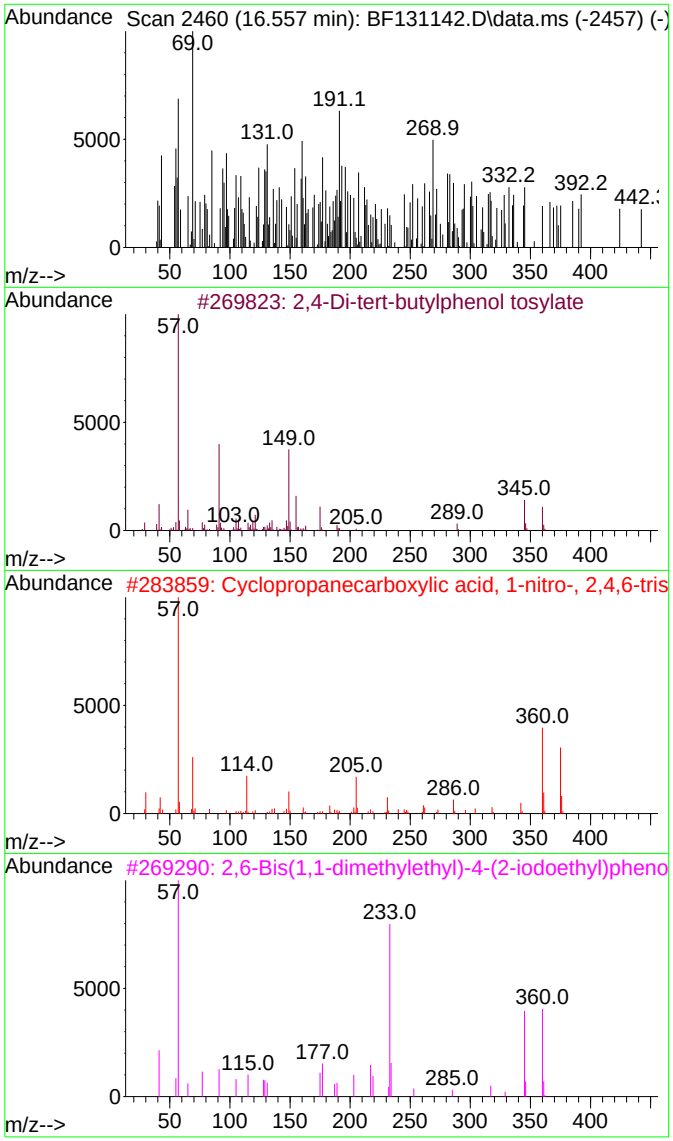
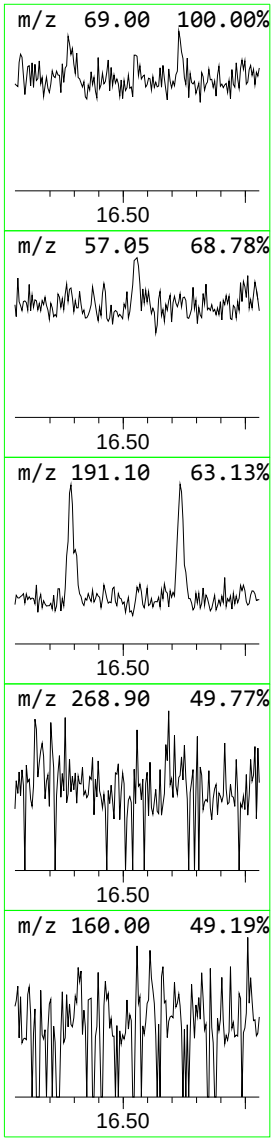
Peak Number 8 unknown16.557 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.557	2.44 ng	31242	Perylene-d12	15.574

Hit# of 3	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Di-tert-butylphenol tosylate	360	C21H28O3S	1071592-64-7	11
2	Cyclopropanecarboxylic acid, 1-n...	375	C22H33NO4	113719-03-2	7
3	2,6-Bis(1,1-dimethylethyl)-4-(2-...	360	C16H25IO	016554-65-7	7





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131142.D
Acq On : 11 Nov 2022 01:16
Operator : CG\JU
Sample : N5491-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.146	30.7	ng	530704	1	6.887	346175	20.0
Propane, 1,1-di...	2.257	2.1	ng	35770	1	6.887	346175	20.0
3-Penten-2-one,...	4.481	2.5	ng	43919	1	6.887	346175	20.0
2-Pentanone, 4-...	5.104	17.5	ng	302453	1	6.887	346175	20.0
Triphenylphosph...	14.169	2.8	ng	54850	5	14.074	389761	20.0
9-Octadecenamid...	14.827	6.9	ng	88190	6	15.574	255900	20.0
Supraene	14.921	4.0	ng	51712	6	15.574	255900	20.0
unknown16.557	16.557	2.4	ng	31242	6	15.574	255900	20.0