LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
Data File : BF139367.D
Acq On : 14 Sep 2024 14:19
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RR-TRIAZINE-WP

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-BF091324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139367.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	10	21	28	rVB	1147272	1845654	78.84%	11.274%
2	3.810	286	292	299	rVB	15013	23912	1.02%	0.146%
3	5.110	503	513	520	rBV	78499	130594	5.58%	0.798%
4	5.504	573	580	585	rBV	1325932	1897744	81.07%	11.592%
5	6.504	743	750	755	rBV	1384357	2006272	85.71%	12.255%
6	6.875	808	813	818	rBV	287881	347590	14.85%	2.123%
7	7.439	902	909	914	rBV	961260	1323155	56.52%	8.082%
8	8.157	1025	1031	1036	rBV	350039	430795	18.40%	2.631%
9	9.233	1208	1214	1219	rBV	1853299	2340888	100.00%	14.299%
10	9.910	1324	1329	1334	rBV	390549	468588	20.02%	2.862%
11	10.133	1361	1367	1379	rVB2	28260	83787	3.58%	0.512%
12	10.627	1445	1451	1455	rBV	125701	163267	6.97%	0.997%
13	10.698	1455	1463	1468	rVV	1103313	1466799	62.66%	8.960%
14	10.980	1506	1511	1514	rBV	141031	168896	7.22%	1.032%
15	11.022	1514	1518	1522	rBV	198322	230337	9.84%	1.407%
16	11.063	1522	1525	1528	rBV	180183	231177	9.88%	1.412%
17	11.092	1528	1530	1532	rBV	145795	172333	7.36%	1.053%
18	11.392	1576	1581	1586	rBV	372388	463786	19.81%	2.833%
19	11.804	1646	1651	1656	rVB	155952	179566	7.67%	1.097%
20	12.074	1693	1697	1700	rBV	21941	23820	1.02%	0.146%
21	12.516	1751	1772	1773	rBV7	8508	36329	1.55%	0.222%
22	12.980	1845	1851	1856	rBV	1391048	1750334	74.77%	10.692%
23	14.027	2024	2029	2035	rBV	206270	254781	10.88%	1.556%
24	15.162	2209	2222	2233	rBV7	12906	50316	2.15%	0.307%
25	15.498	2272	2279	2290	rVB	182847	280086	11.96%	1.711%

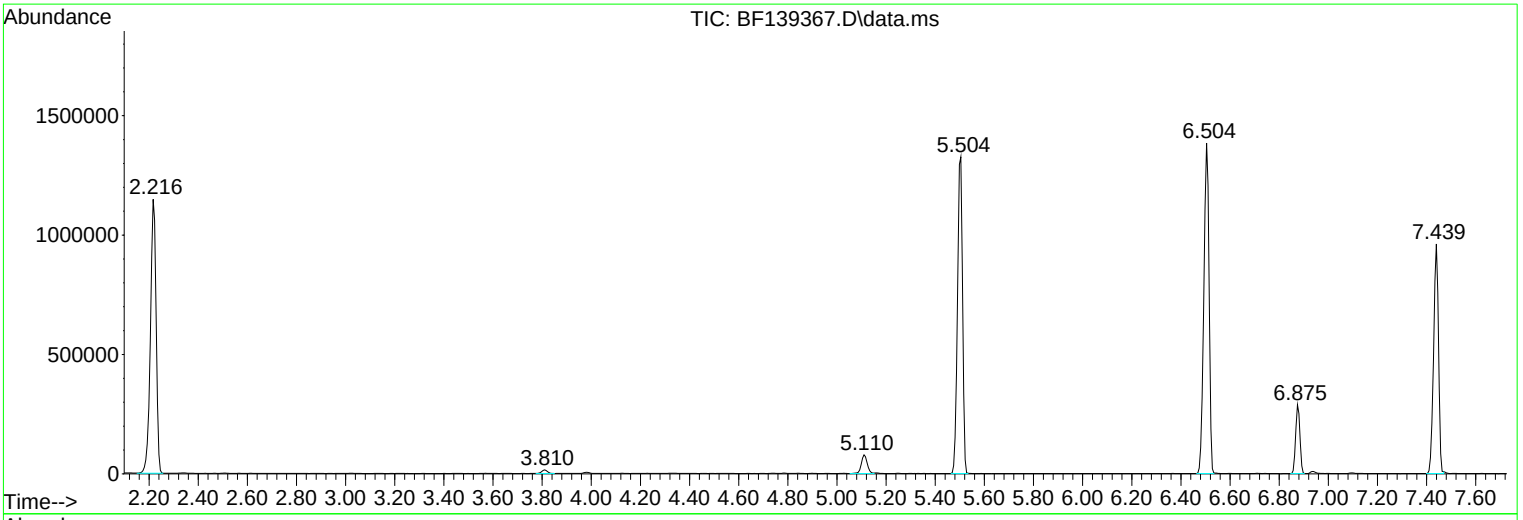
Sum of corrected areas: 16370806

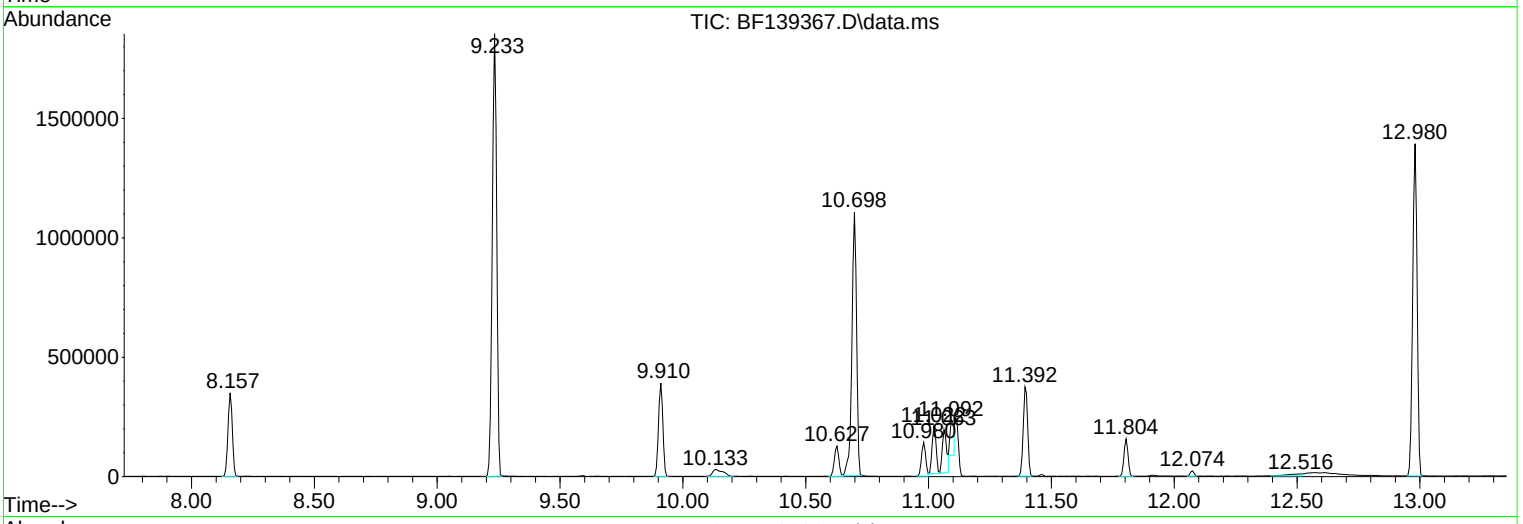
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
Data File : BF139367.D
Acq On : 14 Sep 2024 14:19
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

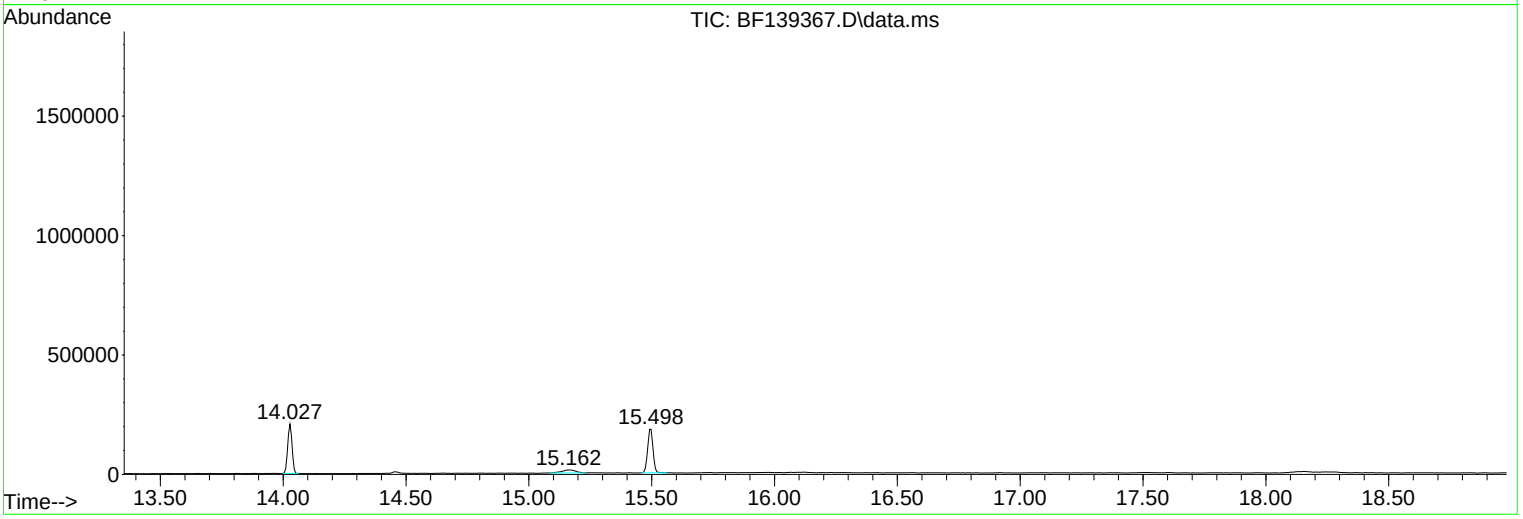
Instrument :
BNA_F
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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\BF091424\
Data File : BF139367.D
Acq On : 14 Sep 2024 14:19
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

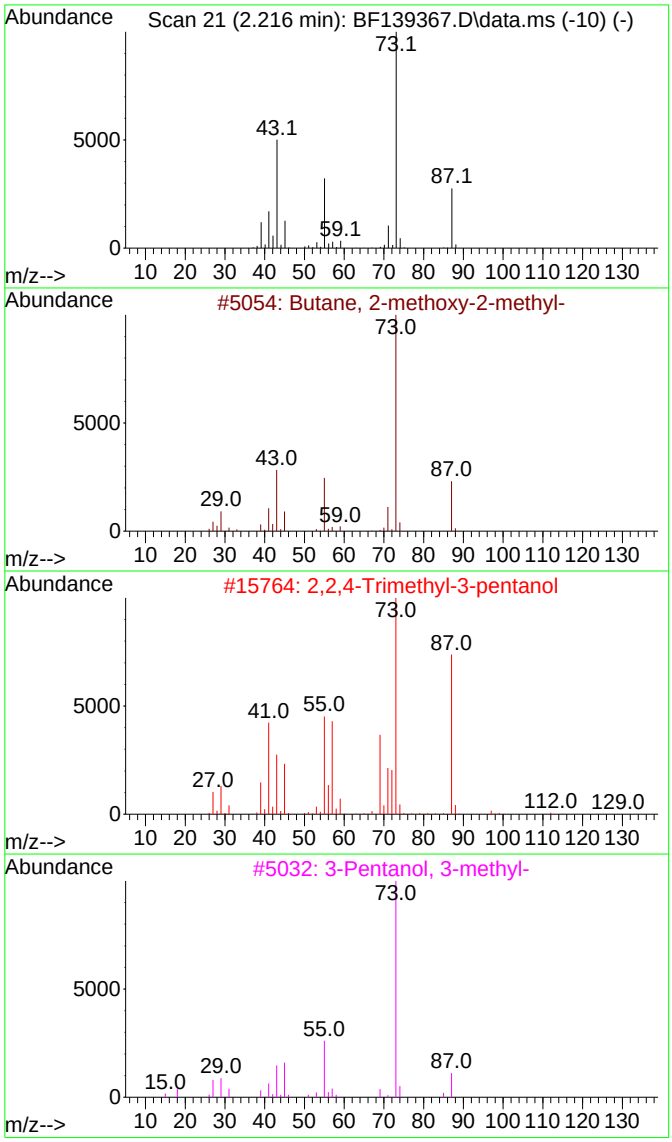
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

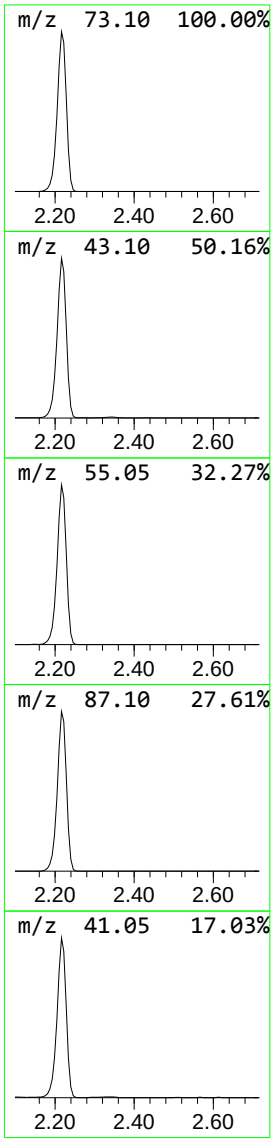
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	106.20 ng	1845650	1,4-Dichlorobenzene-d4	6.875

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	40
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
Data File : BF139367.D
Acq On : 14 Sep 2024 14:19
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RR-TRIAZINE-WP

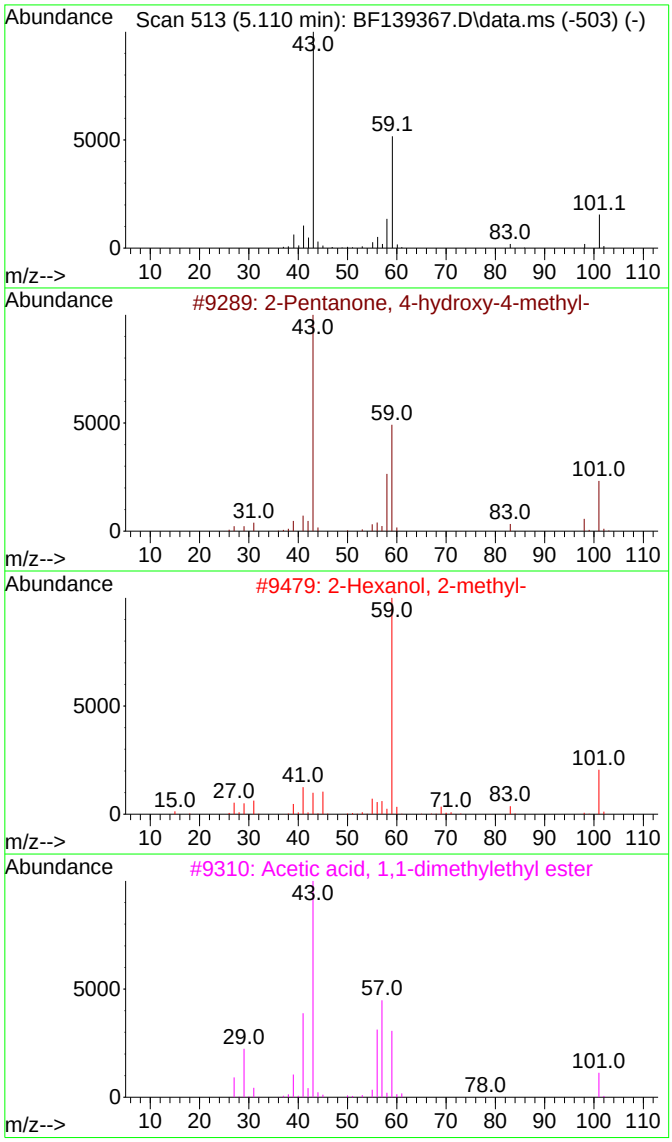
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

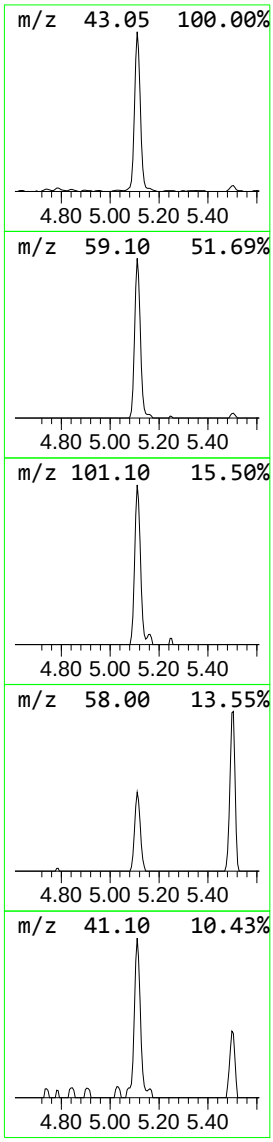
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	7.51 ng	130594	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
Data File : BF139367.D
Acq On : 14 Sep 2024 14:19
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RR-TRIAZINE-WP

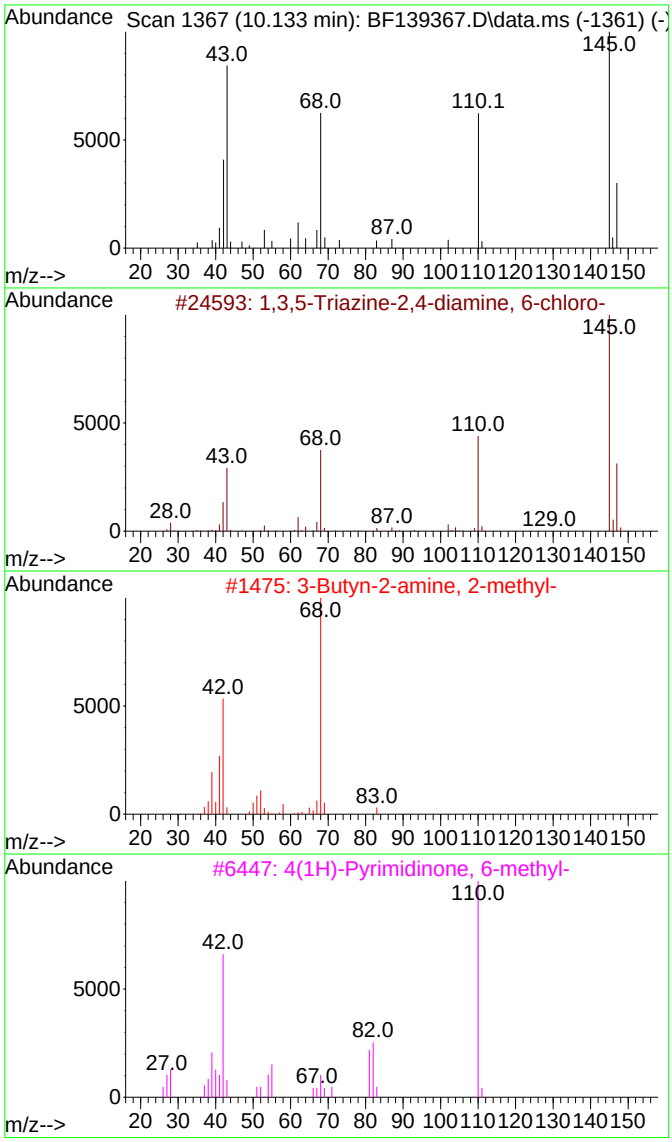
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

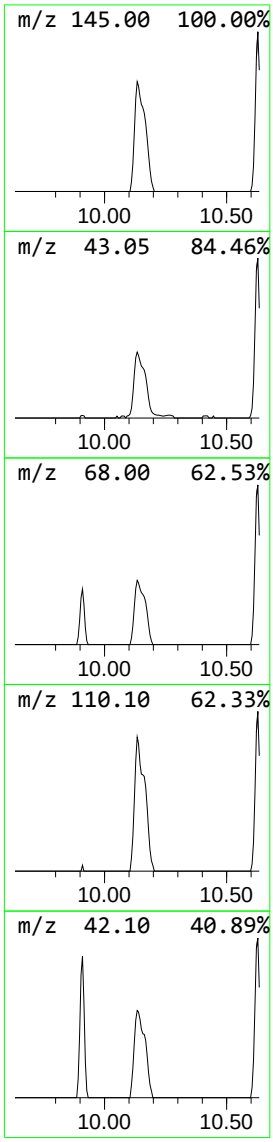
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,3,5-Triazine-2,4-diamine,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.133	3.58 ng	83787	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4-diamine, 6-ch...	145	C3H4ClN5	003397-62-4	91
2	3-Butyn-2-amine, 2-methyl-	83	C5H9N	002978-58-7	14
3	4(1H)-Pyrimidinone, 6-methyl-	110	C5H6N2O	003524-87-6	14
4	2-Chloro-4-fluoroaniline	145	C6H5ClFN	002106-02-7	9
5	4-Chloro-2-fluoroaniline	145	C6H5ClFN	057946-56-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
Data File : BF139367.D
Acq On : 14 Sep 2024 14:19
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

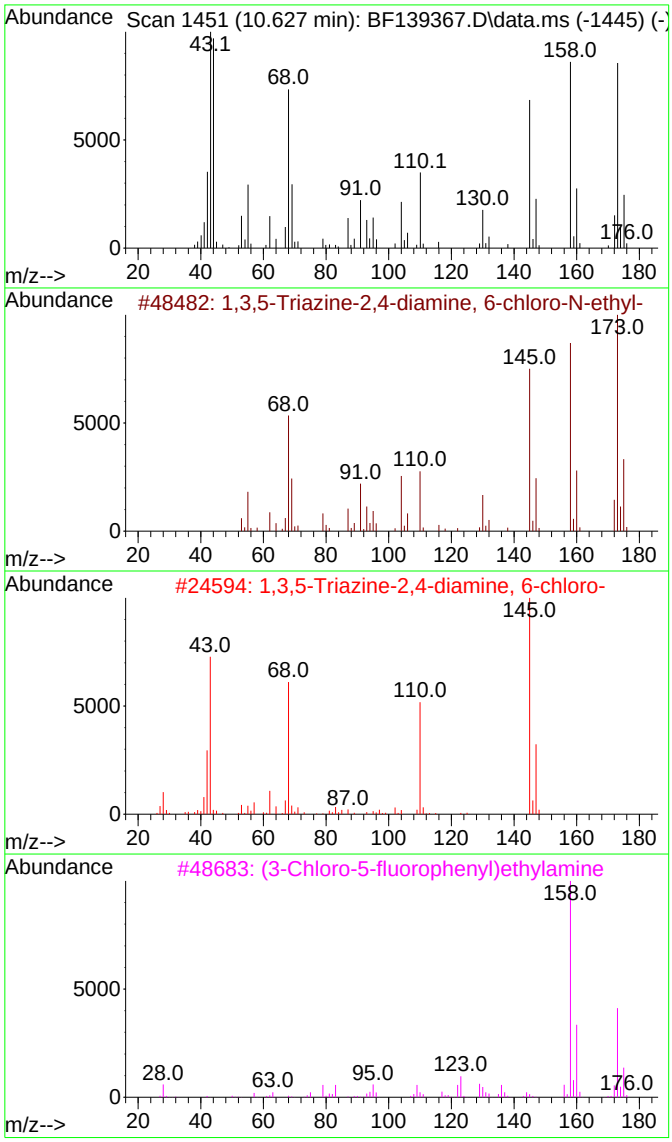
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

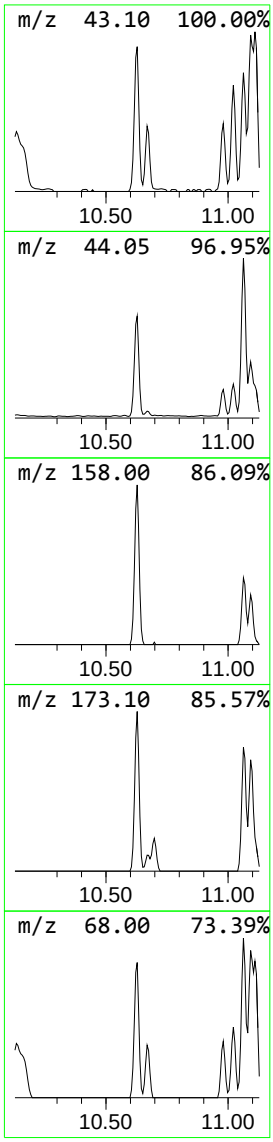
****

Peak Number 4 unknown10.628 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.628	6.97 ng	163267	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4-diamine, 6-ch...	173	C5H8ClN5	001007-28-9	98
2	1,3,5-Triazine-2,4-diamine, 6-ch...	145	C3H4ClN5	003397-62-4	47
3	(3-Chloro-5-fluorophenyl)ethylamine	173	C8H9ClFN	1000306-63-1	46
4	2-Methylthio-4-chloroaniline	173	C7H8ClNS	029690-21-9	43
5	3-Chloro-N-(1,1-dimethylpropynyl...	173	C8H12ClNO	039109-07-4	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
Data File : BF139367.D
Acq On : 14 Sep 2024 14:19
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

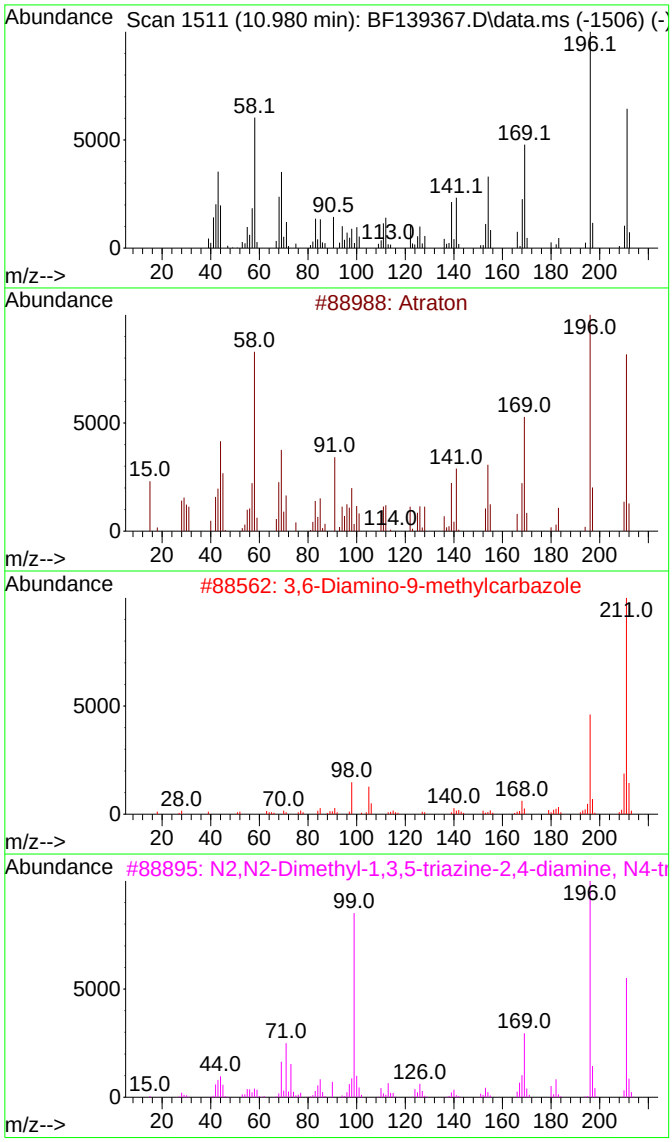
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

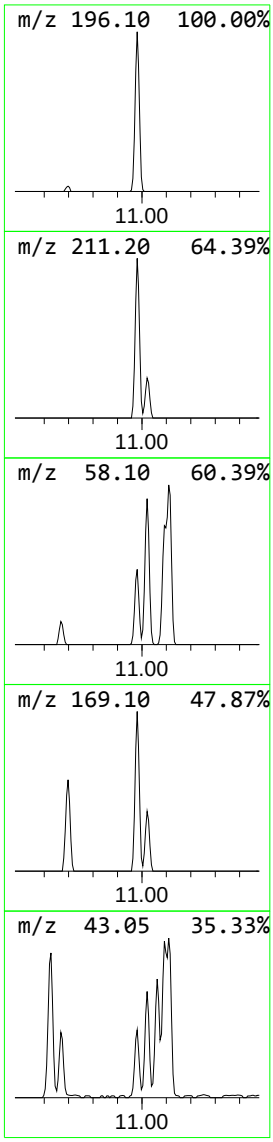
****

Peak Number 5 Atraton Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.980	7.28 ng	168896	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Atraton	211	C9H17N5O	001610-17-9	90
2	3,6-Diamino-9-methylcarbazole	211	C13H13N3	046498-17-3	45
3	N2,N2-Dimethyl-1,3,5-triazine-2,...	211	C8H17N5Si	1000471-09-5	45
4	Xanthone	196	C13H8O2	000090-47-1	42
5	2(1H)-Pyrimidinone,1,5-dimethyl-...	211	C9H17N3OSi	1000147-48-1	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
Data File : BF139367.D
Acq On : 14 Sep 2024 14:19
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

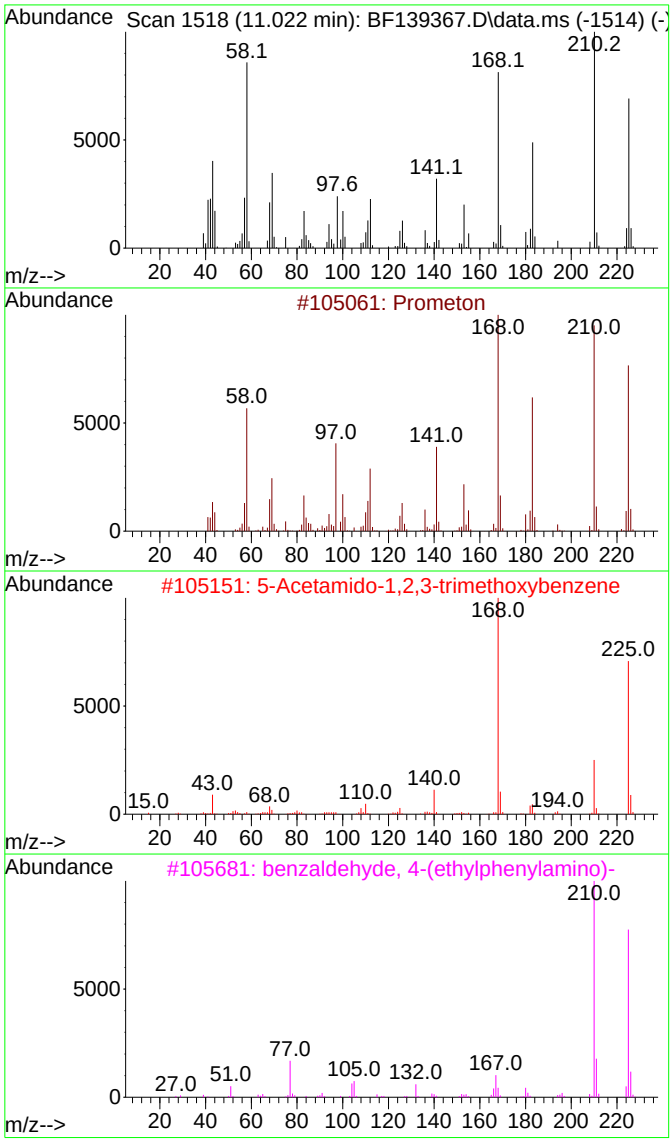
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

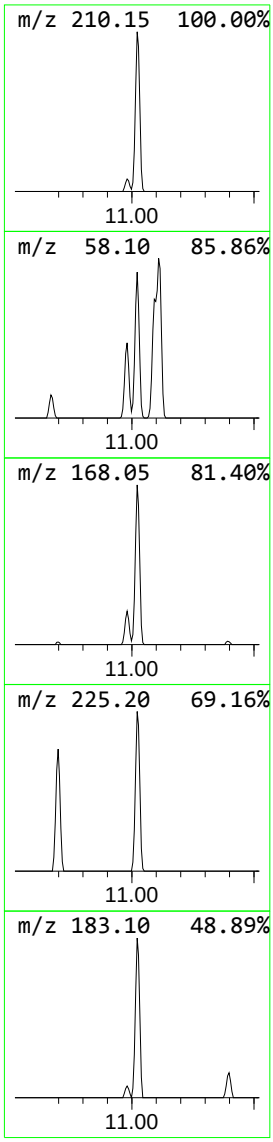
****

Peak Number 6 Prometon Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.022	9.93 ng	230337	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Prometon	225	C10H19N5O	001610-18-0	97
2	5-Acetamido-1,2,3-trimethoxybenzene	225	C11H15NO4	004304-24-9	22
3	benzaldehyde, 4-(ethylphenylamino)-	225	C15H15NO	1000400-90-8	18
4	Terbumeton	225	C10H19N5O	033693-04-8	14
5	4-Fluoroaniline, N-trimethylsilyl-	183	C9H14FNSi	033407-00-0	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
Data File : BF139367.D
Acq On : 14 Sep 2024 14:19
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

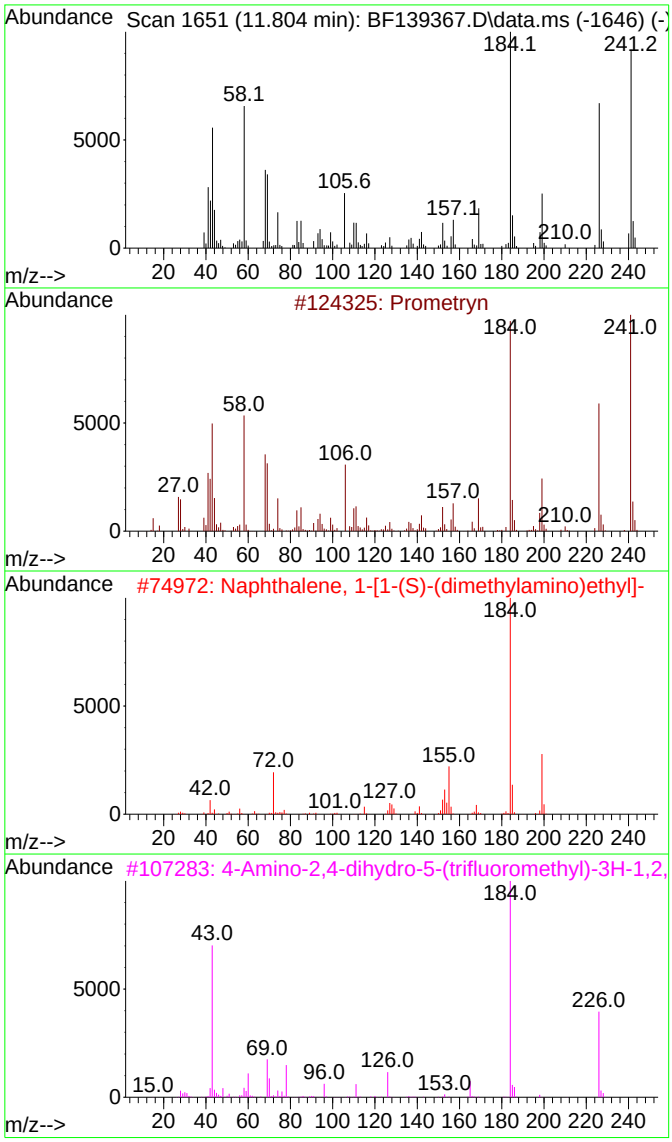
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

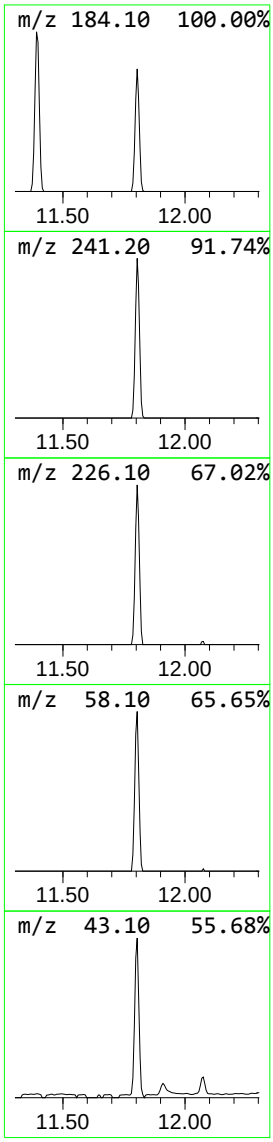
****

Peak Number 7 Prometryn Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	7.74 ng	179566	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Prometryn	241	C10H19N5S	007287-19-6	99
2	Naphthalene, 1-[1-(S)-(dimethyla...	199	C14H17N	1010163-58-5	38
3	4-Amino-2,4-dihydro-5-(trifluoro...	226	C5H5F3N4OS	1010479-88-8	35
4	Ethanone, 1-(10H-phenothiazin-2-...	241	C14H11NOS	006631-94-3	25
5	Benzenesulfonamide, 4-acetyl-	199	C8H9NO3S	001565-17-9	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
Data File : BF139367.D
Acq On : 14 Sep 2024 14:19
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

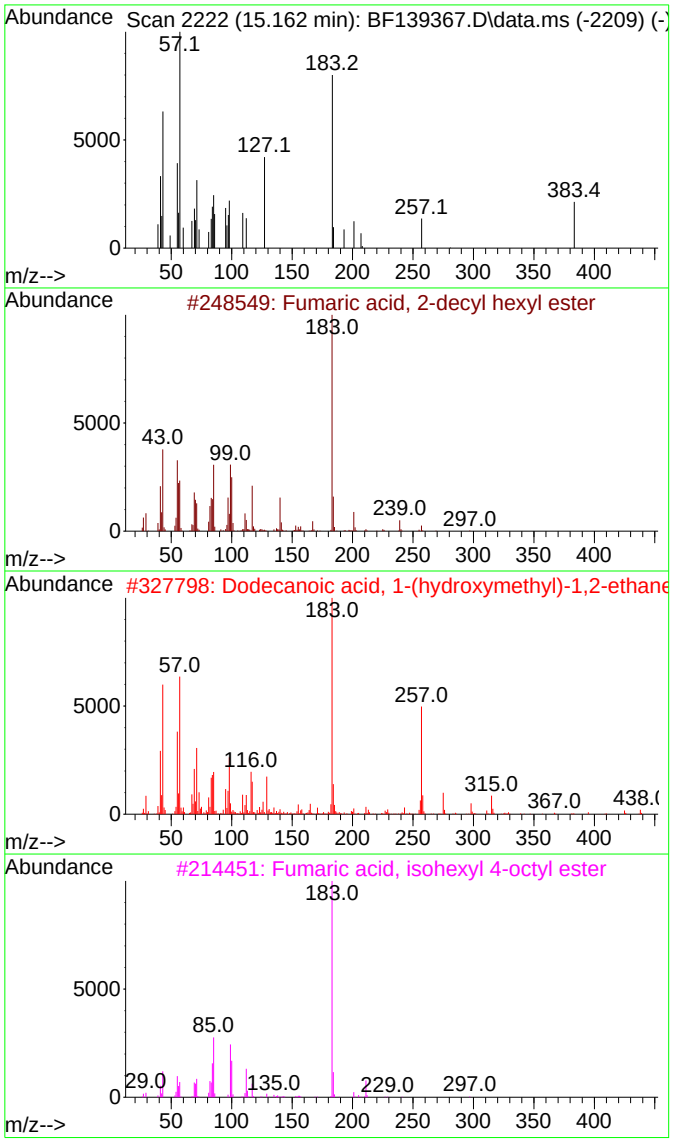
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

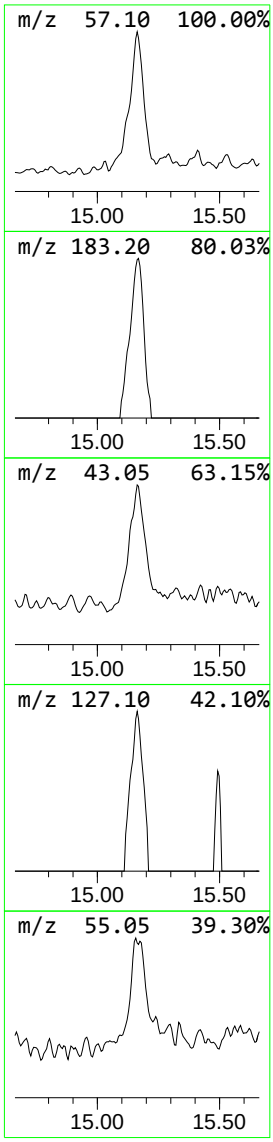
****

Peak Number 8 unknown15.163 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	3.59 ng	50316	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 2-decyl hexyl ester	340	C20H36O4	1000348-58-9	47
2	Dodecanoic acid, 1-(hydroxymethy...	456	C27H52O5	017598-94-6	43
3	Fumaric acid, isohexyl 4-octyl e...	312	C18H32O4	1000339-21-6	43
4	Dodecanoic acid, ethenyl ester	226	C14H26O2	002146-71-6	38
5	Lauric anhydride	382	C24H46O3	000645-66-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091424\
Data File : BF139367.D
Acq On : 14 Sep 2024 14:19
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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...	2.216	106.2	ng	1845650	1	6.875	347590	20.0
2-Pentanone, 4-...	5.110	7.5	ng	130594	1	6.875	347590	20.0
1,3,5-Triazine-...	10.133	3.6	ng	83787	3	9.910	468588	20.0
unknown10.628	10.628	7.0	ng	163267	3	9.910	468588	20.0
Atraton	10.980	7.3	ng	168896	4	11.392	463786	20.0
Prometon	11.022	9.9	ng	230337	4	11.392	463786	20.0
Prometryn	11.804	7.7	ng	179566	4	11.392	463786	20.0
unknown15.163	15.163	3.6	ng	50316	6	15.498	280086	20.0