LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130029.D
Acq On : 26 Aug 2022 20:55
Operator : CG\JU
Sample : N4379-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-X

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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130029.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.975	454	457	471	rBV	83725	121599	4.50%	0.646%
2	5.393	524	528	551	rBV	2518028	2690204	99.54%	14.292%
3	6.410	698	701	724	rBV	2562134	2582435	95.55%	13.719%
4	6.745	755	758	766	rVB	854603	698856	25.86%	3.713%
5	7.316	852	855	866	rBV	1736207	1636467	60.55%	8.694%
6	8.028	973	976	984	rBV	1026623	825754	30.55%	4.387%
7	9.104	1155	1159	1162	rBV	3251713	2702622	100.00%	14.358%
8	9.781	1271	1274	1278	rBV	923561	734546	27.18%	3.902%
9	10.575	1406	1409	1423	rBV	1412105	1318029	48.77%	7.002%
10	11.269	1524	1527	1531	rBV	788383	665335	24.62%	3.535%
11	11.792	1612	1616	1620	rBV3	28802	36530	1.35%	0.194%
12	12.657	1760	1763	1768	rBV	477020	376051	13.91%	1.998%
13	12.857	1792	1797	1802	rBV	2627909	2626351	97.18%	13.953%
14	13.804	1951	1958	1968	rBV4	68756	234648	8.68%	1.247%
15	13.916	1974	1977	1985	rVB	724556	687189	25.43%	3.651%
16	14.004	1989	1992	1996	rVV	70365	64630	2.39%	0.343%
17	14.051	1998	2000	2004	rVB	39386	34820	1.29%	0.185%
18	14.357	2049	2052	2057	rBV	53307	55960	2.07%	0.297%
19	14.521	2077	2080	2082	rBV	41097	34503	1.28%	0.183%
20	14.657	2100	2103	2108	rVB	44657	46576	1.72%	0.247%
21	14.974	2154	2157	2160	rVB	50934	54902	2.03%	0.292%
22	15.333	2215	2218	2220	rBV	44443	51243	1.90%	0.272%
23	15.363	2220	2223	2228	rVB	404607	487126	18.02%	2.588%
24	15.739	2285	2287	2292	rVB2	44947	57015	2.11%	0.303%

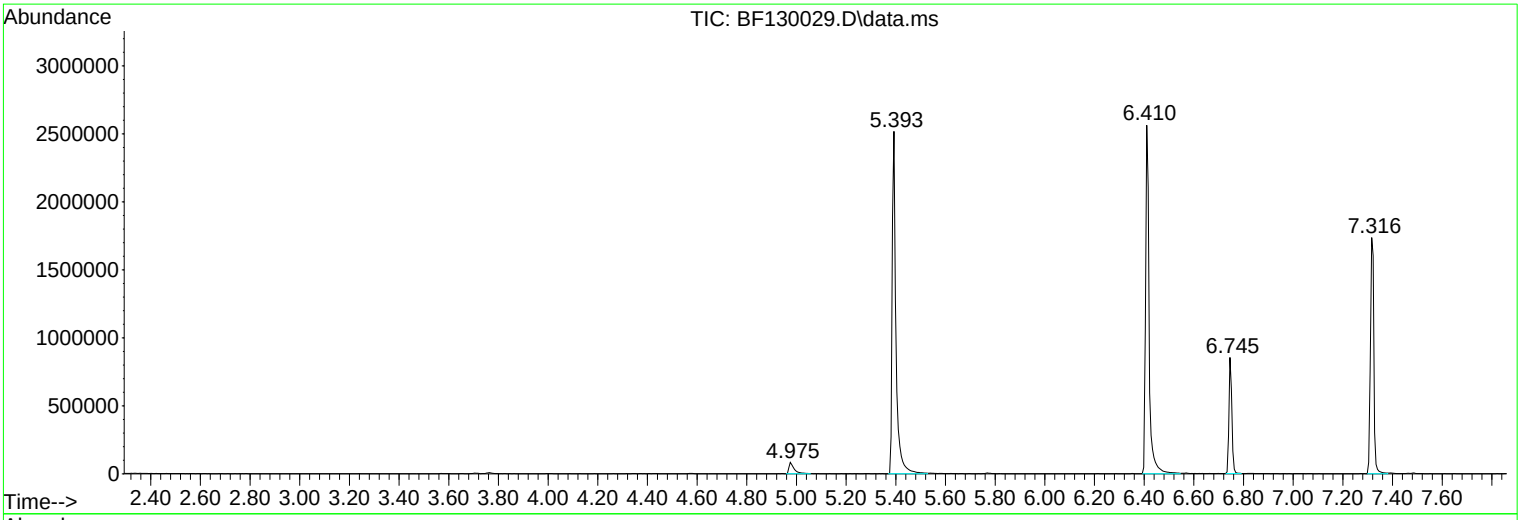
Sum of corrected areas: 18823391

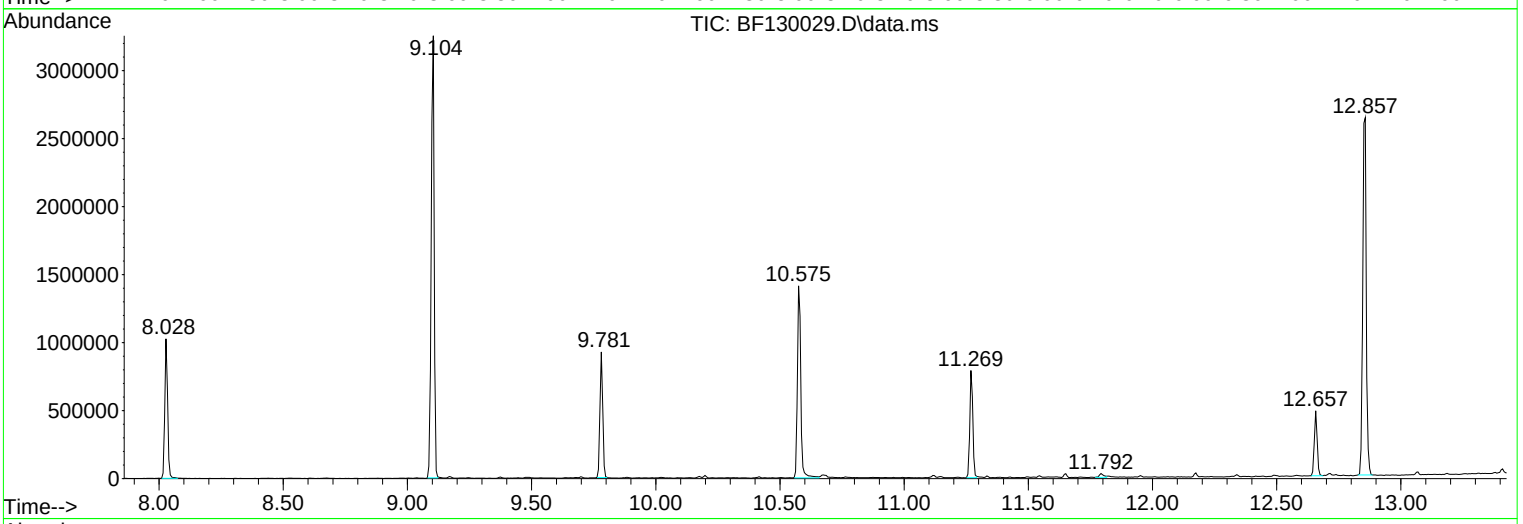
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130029.D
Acq On : 26 Aug 2022 20:55
Operator : CG\JU
Sample : N4379-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

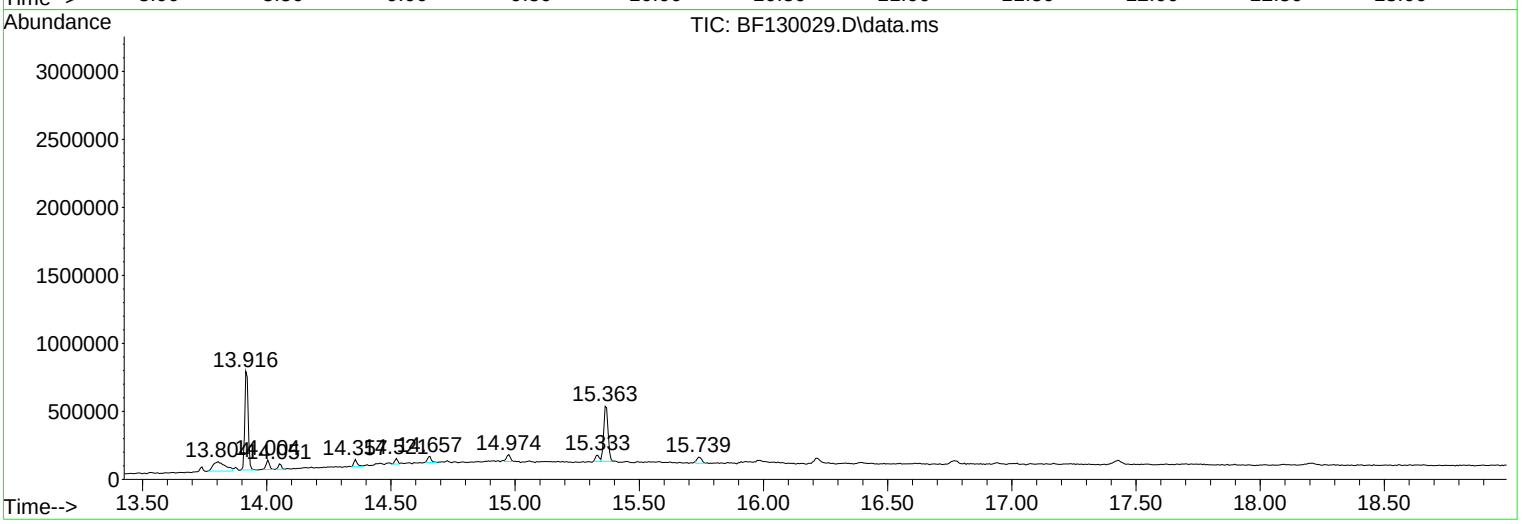
Instrument :
BNA_F
ClientSampleId :
DUP-X

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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\BF082622\
Data File : BF130029.D
Acq On : 26 Aug 2022 20:55
Operator : CG\JU
Sample : N4379-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-X

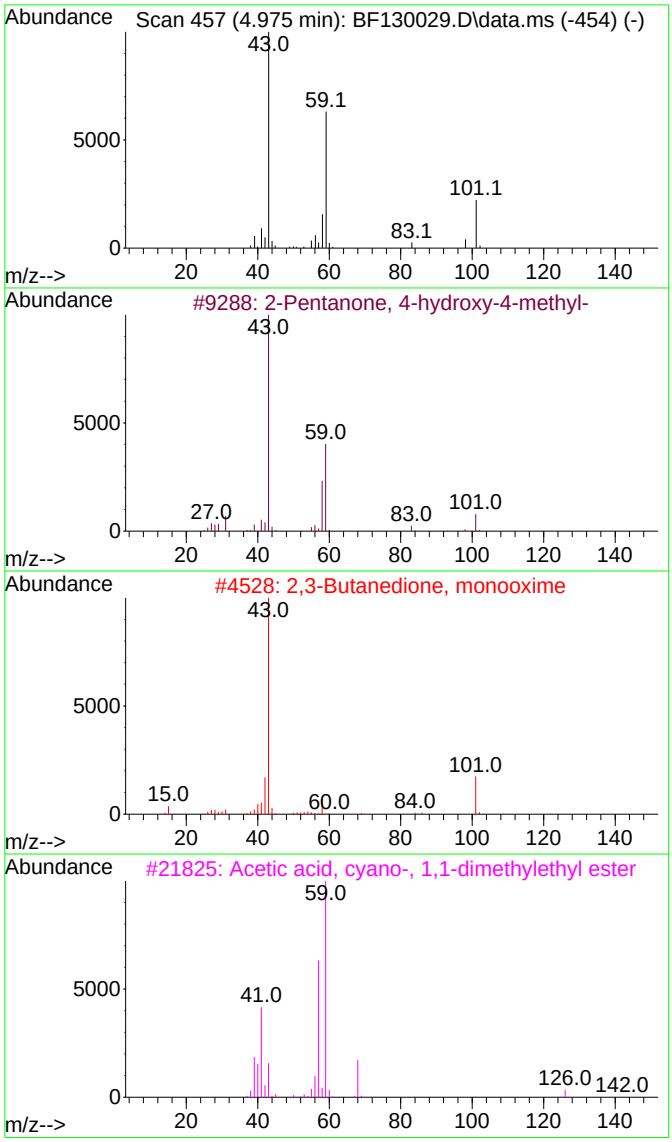
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

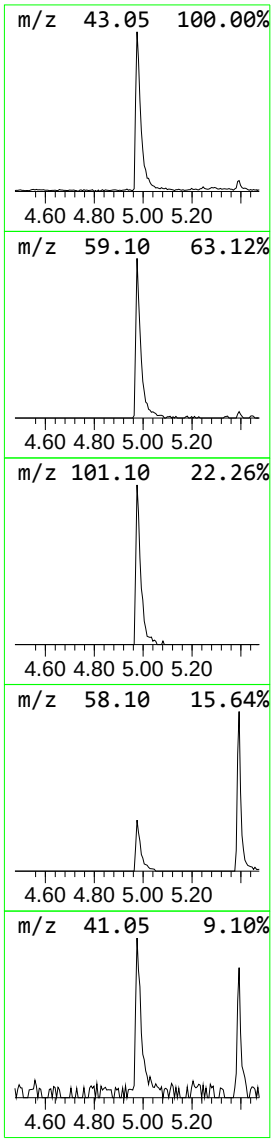
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.975	3.48 ng	121599	1,4-Dichlorobenzene-d4	6.745

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Guanidine	59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130029.D
Acq On : 26 Aug 2022 20:55
Operator : CG\JU
Sample : N4379-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-X

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

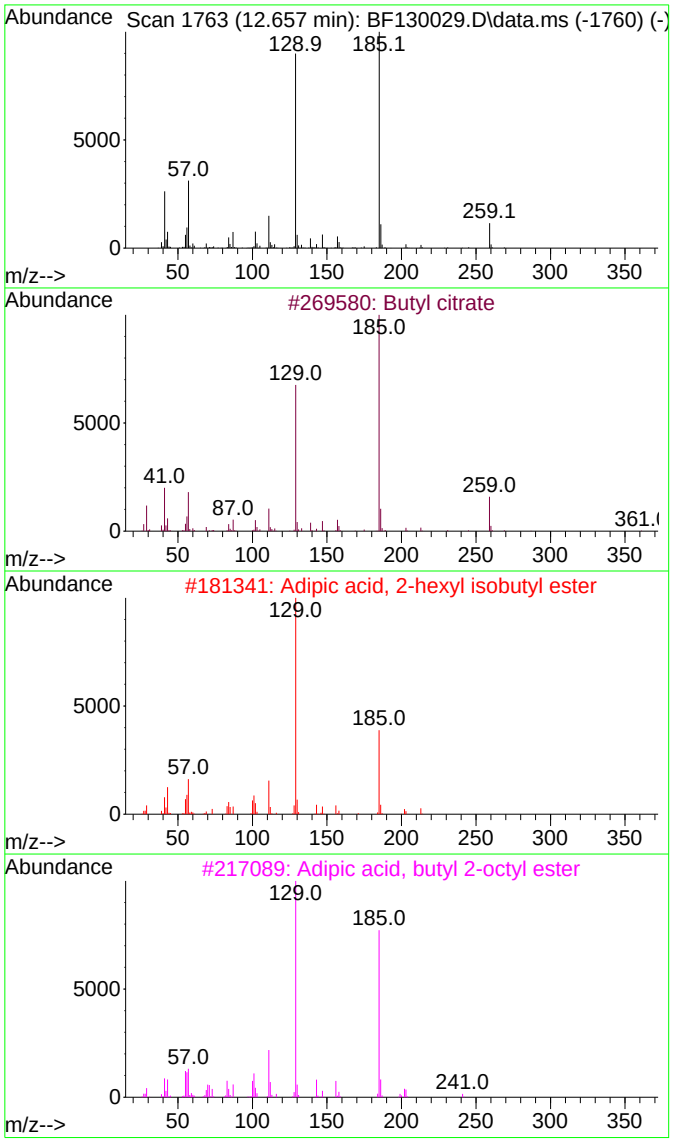
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

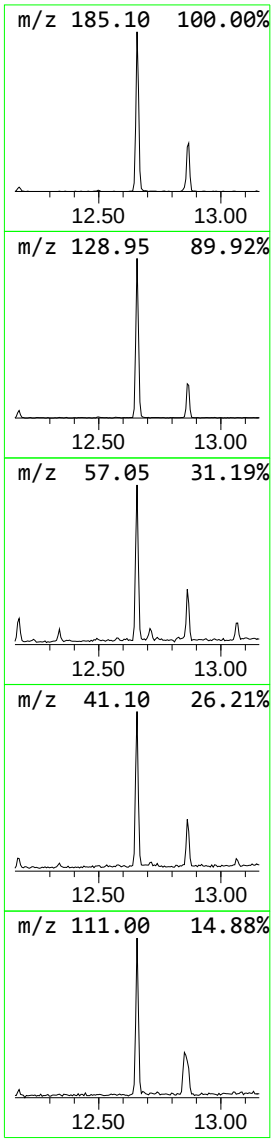
****

Peak Number 2 Butyl citrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.657	10.94 ng	376051	Chrysene-d12	13.921

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	91
2	Adipic acid, 2-hexyl isobutyl ester	286	C16H30O4	1000353-70-9	78
3	Adipic acid, butyl 2-octyl ester	314	C18H34O4	1010324-44-6	64
4	Adipic acid, 2-ethylcyclohexyl i...	312	C18H32O4	1000324-22-5	64
5	Dibutyl adipate	258	C14H26O4	000105-99-7	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130029.D
Acq On : 26 Aug 2022 20:55
Operator : CG\JU
Sample : N4379-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-X

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

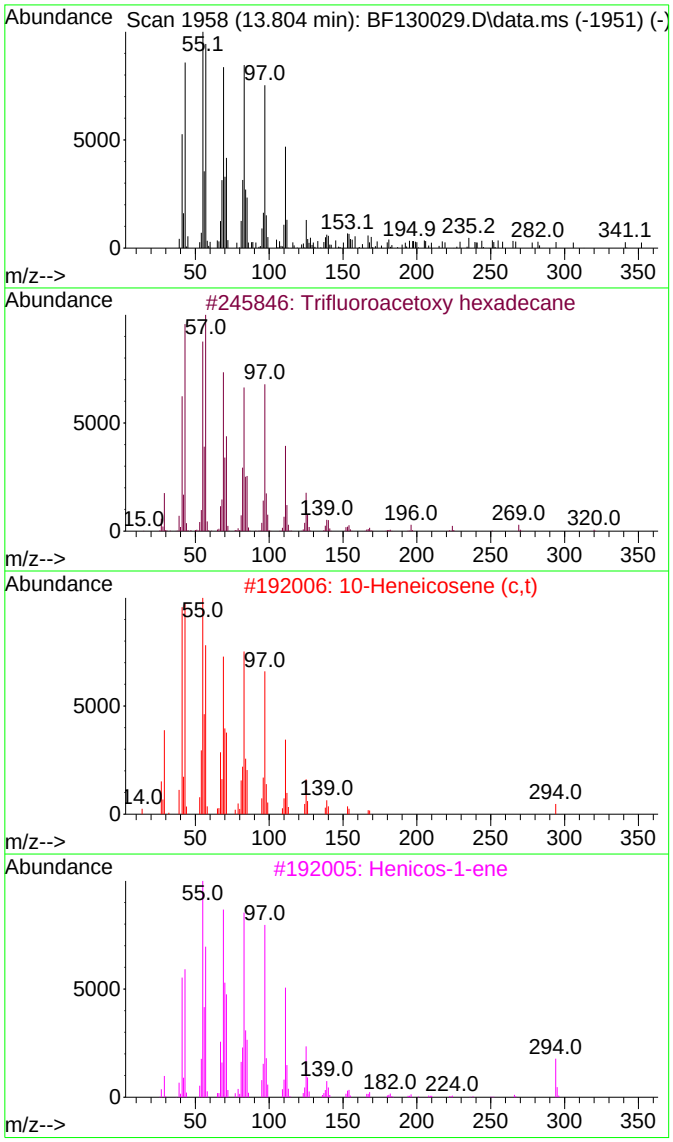
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

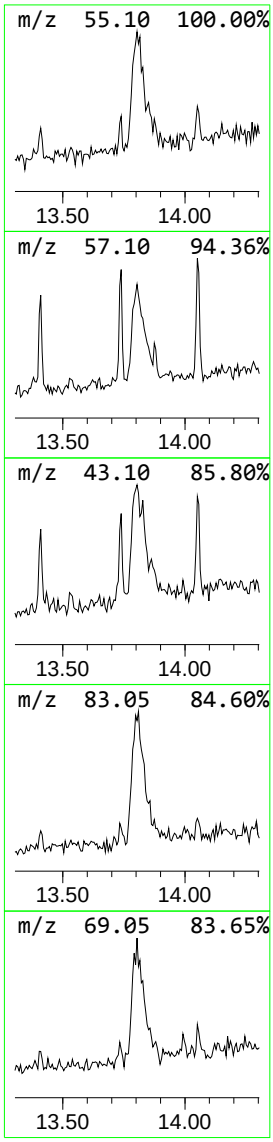
****

Peak Number 3 Trifluoroacetoxy hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	6.83 ng	234648	Chrysene-d12	13.921

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	10-Heneicosene (c,t)	294	C21H42	095008-11-0	93
3	Henicos-1-ene	294	C21H42	001599-68-4	91
4	1-Tetracosene	336	C24H48	010192-32-2	91
5	Cyclopentadecane	210	C15H30	000295-48-7	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130029.D
Acq On : 26 Aug 2022 20:55
Operator : CG\JU
Sample : N4379-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-X

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

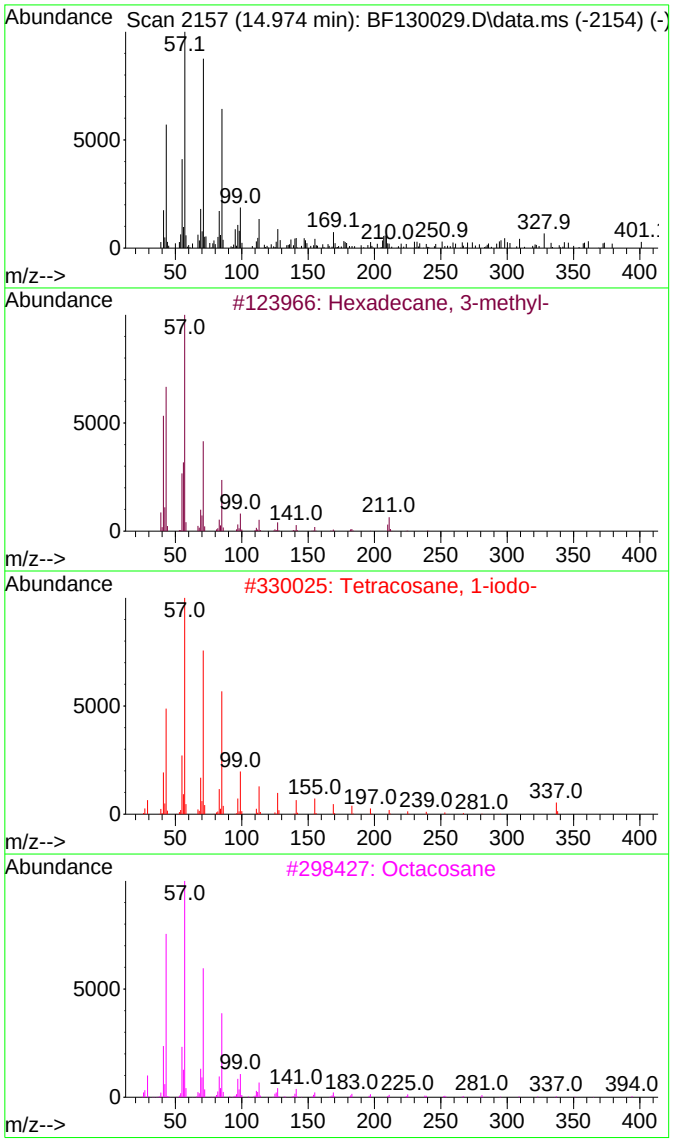
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

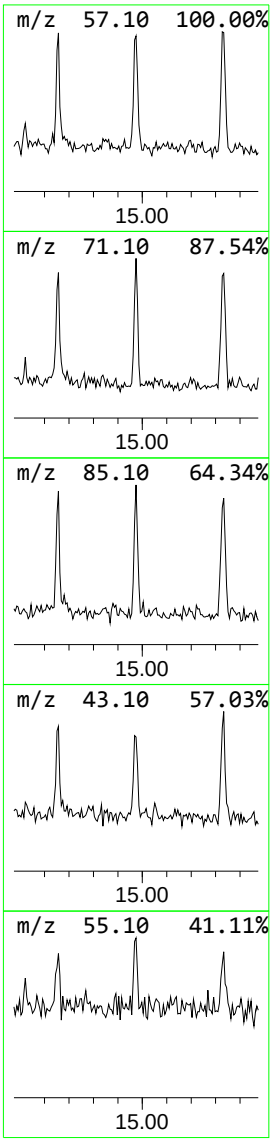
****

Peak Number 4 Hexadecane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	2.25 ng	54902	Perylene-d12	15.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	76
2	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	68
3	Octacosane	394	C28H58	000630-02-4	68
4	Nonadecane	268	C19H40	000629-92-5	64
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130029.D
Acq On : 26 Aug 2022 20:55
Operator : CG\JU
Sample : N4379-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-X

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

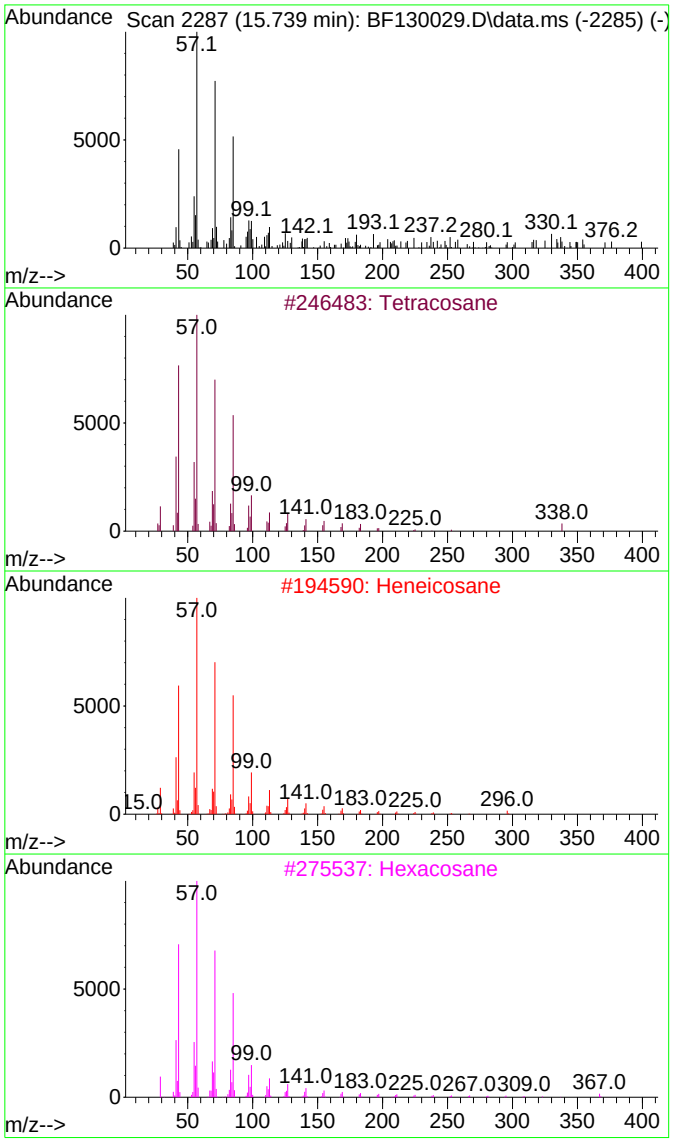
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

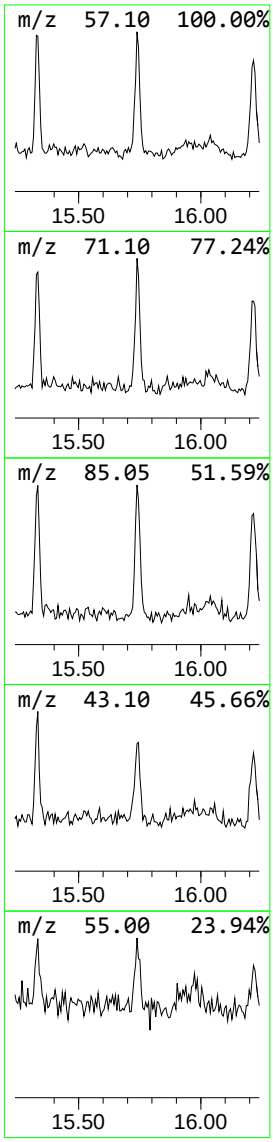
****

Peak Number 5 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.739	2.34 ng	57015	Perylene-d12	15.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	89
2	Heneicosane	296	C21H44	000629-94-7	89
3	Hexacosane	366	C26H54	000630-01-3	64
4	Octacosane	394	C28H58	000630-02-4	64
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130029.D
Acq On : 26 Aug 2022 20:55
Operator : CG\JU
Sample : N4379-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-X

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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
2-Pentanone, 4-...	4.975	3.5	ng	121599	1	6.745	698856	20.0
Butyl citrate	12.657	10.9	ng	376051	5	13.921	687189	20.0
Trifluoroacetox...	13.804	6.8	ng	234648	5	13.921	687189	20.0
Hexadecane, 3-m...	14.974	2.3	ng	54902	6	15.363	487126	20.0
Tetracosane	15.739	2.3	ng	57015	6	15.363	487126	20.0