LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081522\
Data File : BF129791.D
Acq On : 15 Aug 2022 20:47
Operator : CG\JU
Sample : N4200-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S9

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: BF129791.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	465	468	481	rVB	741752	871304	24.51%	3.444%
2	5.463	536	540	557	rBV	2630433	2529098	71.14%	9.996%
3	6.475	708	712	726	rBV	2927557	2629032	73.95%	10.391%
4	6.822	767	771	775	rBV	1065826	933731	26.26%	3.691%
5	7.386	863	867	876	rBV	1853736	1788635	50.31%	7.069%
6	8.104	984	989	993	rBV	1544613	1298327	36.52%	5.132%
7	9.180	1166	1172	1175	rBV	3884528	3523221	99.10%	13.925%
8	9.857	1283	1287	1291	rBV	1779746	1546025	43.49%	6.111%
9	10.657	1419	1423	1426	rBV	2226624	2093214	58.88%	8.273%
10	11.351	1537	1541	1544	rBV	1886747	1567924	44.10%	6.197%
11	12.568	1744	1748	1753	rBV	72177	64026	1.80%	0.253%
12	12.798	1781	1787	1793	rBV	71857	75209	2.12%	0.297%
13	12.939	1806	1811	1814	rBV	3679671	3555203	100.00%	14.052%
14	13.886	1964	1972	1982	rBV8	41529	176623	4.97%	0.698%
15	13.998	1987	1991	1995	rBV	1192682	1078328	30.33%	4.262%
16	14.886	2139	2142	2147	rBV	146079	147687	4.15%	0.584%
17	15.074	2171	2174	2177	rVB2	82233	86133	2.42%	0.340%
18	15.209	2191	2197	2201	rBV9	16749	43316	1.22%	0.171%
19	15.468	2234	2241	2254	rVB	670204	859772	24.18%	3.398%
20	15.651	2268	2272	2277	rBV2	40325	58712	1.65%	0.232%
21	15.874	2305	2310	2317	rVB	111155	164055	4.61%	0.648%
22	16.662	2440	2444	2451	rVB6	26906	49077	1.38%	0.194%
23	16.951	2487	2493	2502	rVB3	56413	123097	3.46%	0.487%
24	17.639	2604	2610	2614	rBV9	15769	39037	1.10%	0.154%

Sum of corrected areas: 25300786

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ALS Vial : 11 Sample Multiplier: 1

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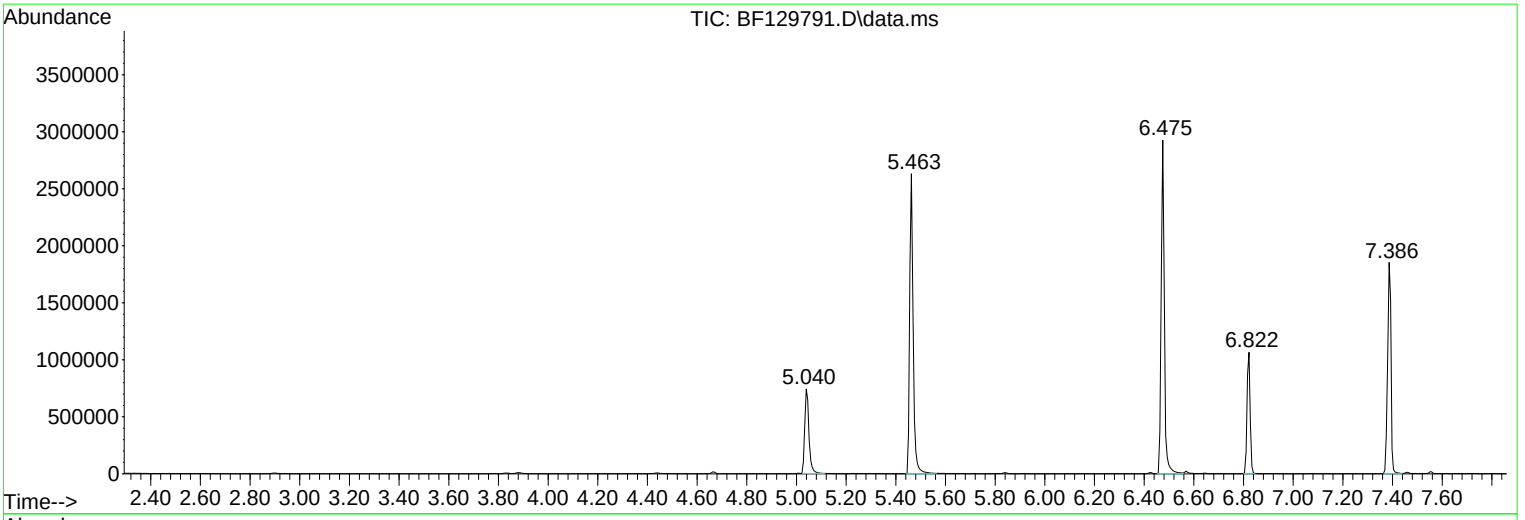
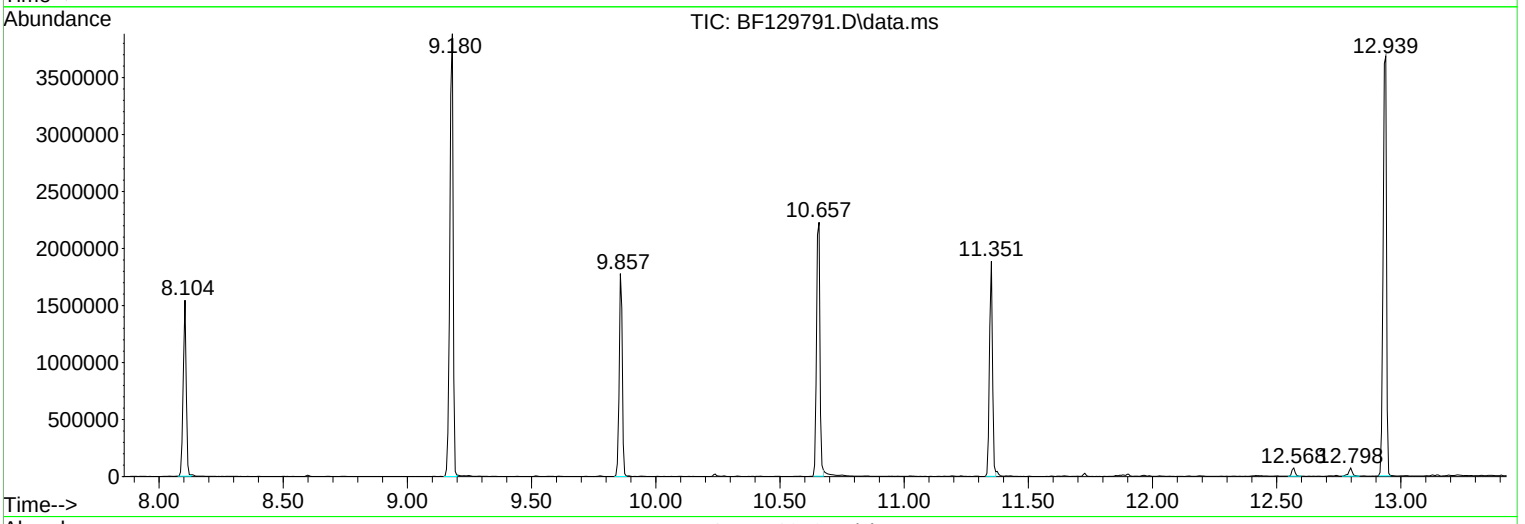
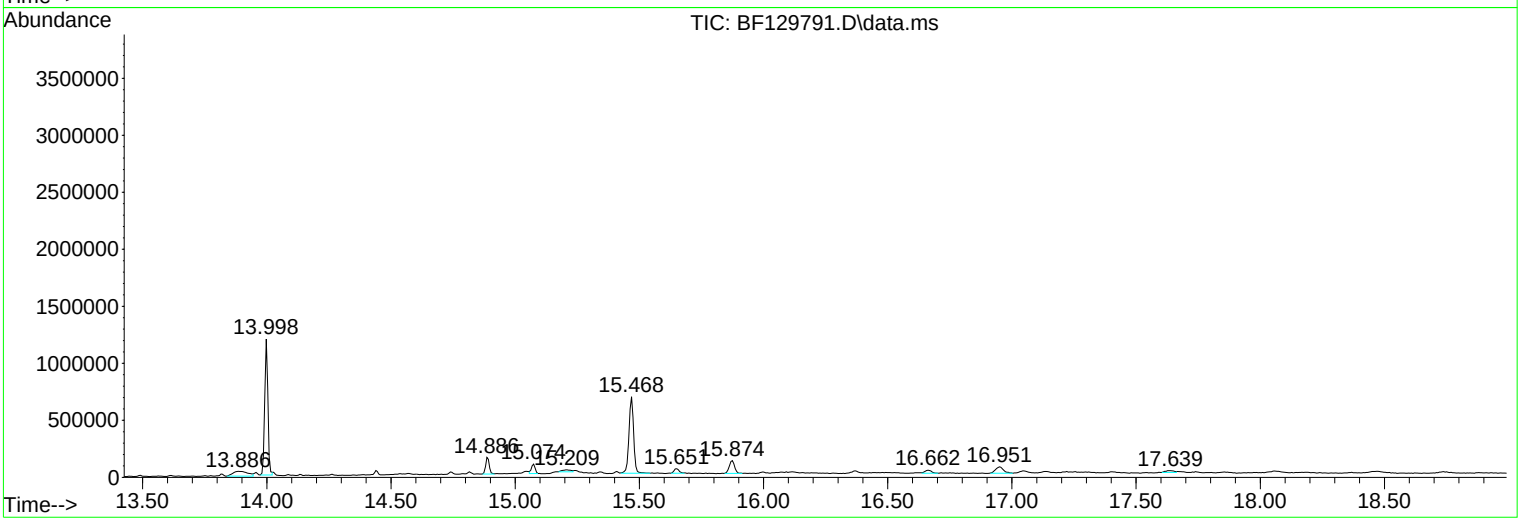
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Data File : BF129791.D
Acq On : 15 Aug 2022 20:47
Operator : CG\JU
Sample : N4200-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

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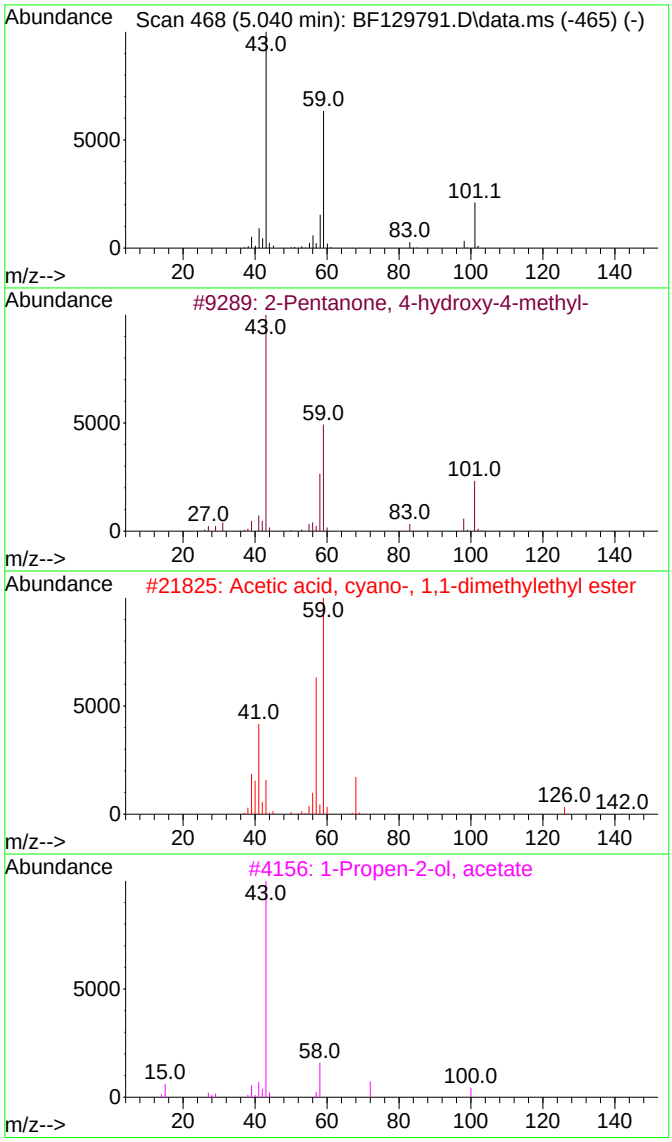
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

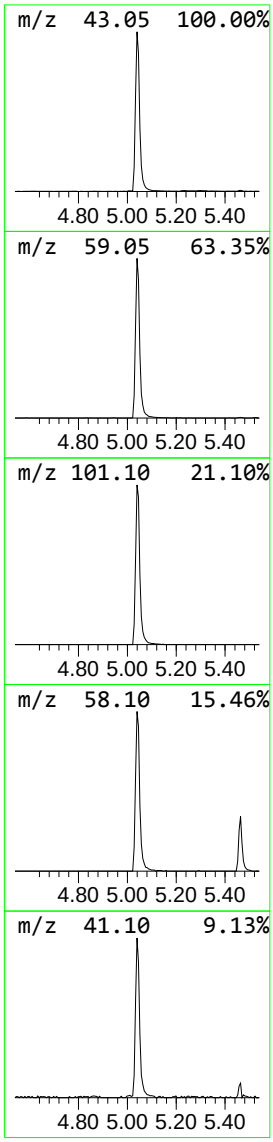
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	18.66 ng	871304	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081522\
Data File : BF129791.D
Acq On : 15 Aug 2022 20:47
Operator : CG\JU
Sample : N4200-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S9

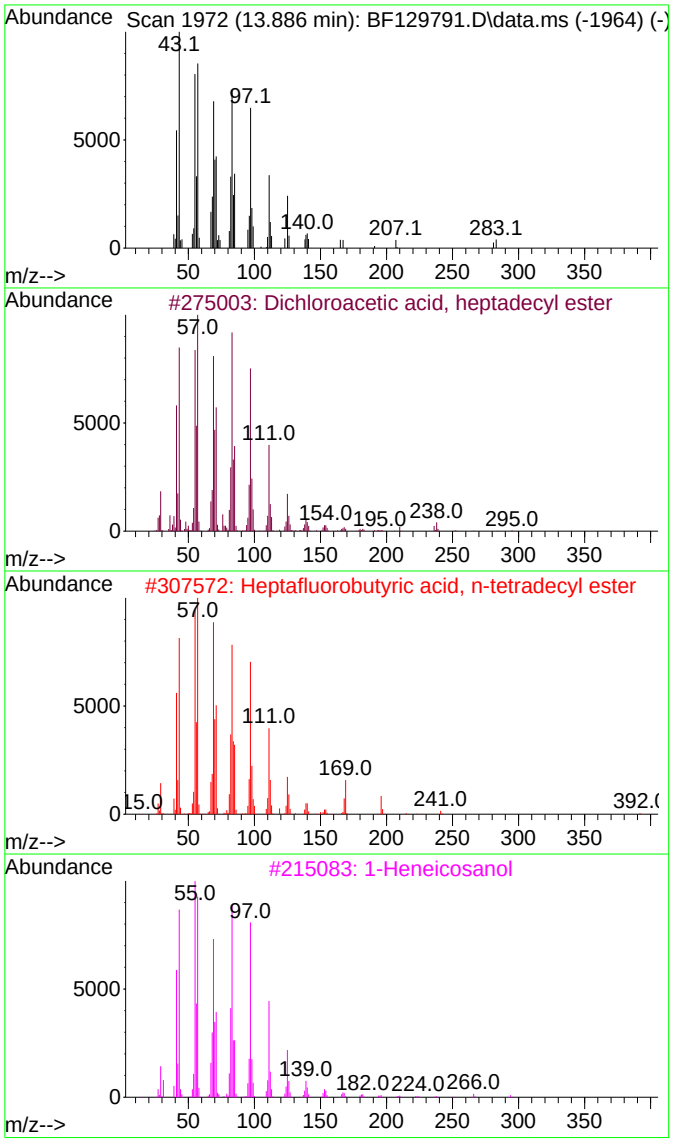
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

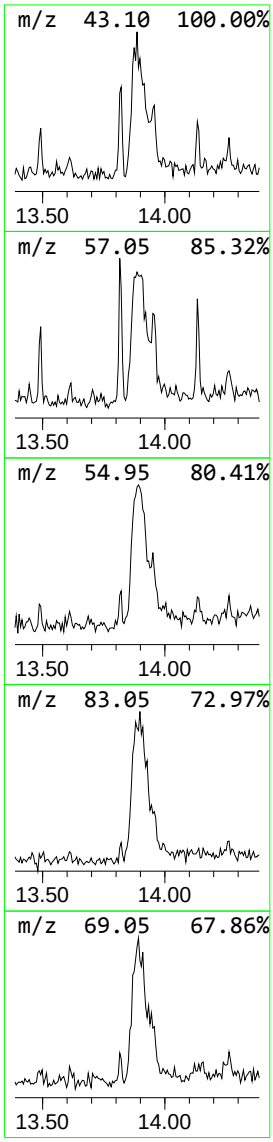
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	3.28 ng	176623	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081522\
Data File : BF129791.D
Acq On : 15 Aug 2022 20:47
Operator : CG\JU
Sample : N4200-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S9

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

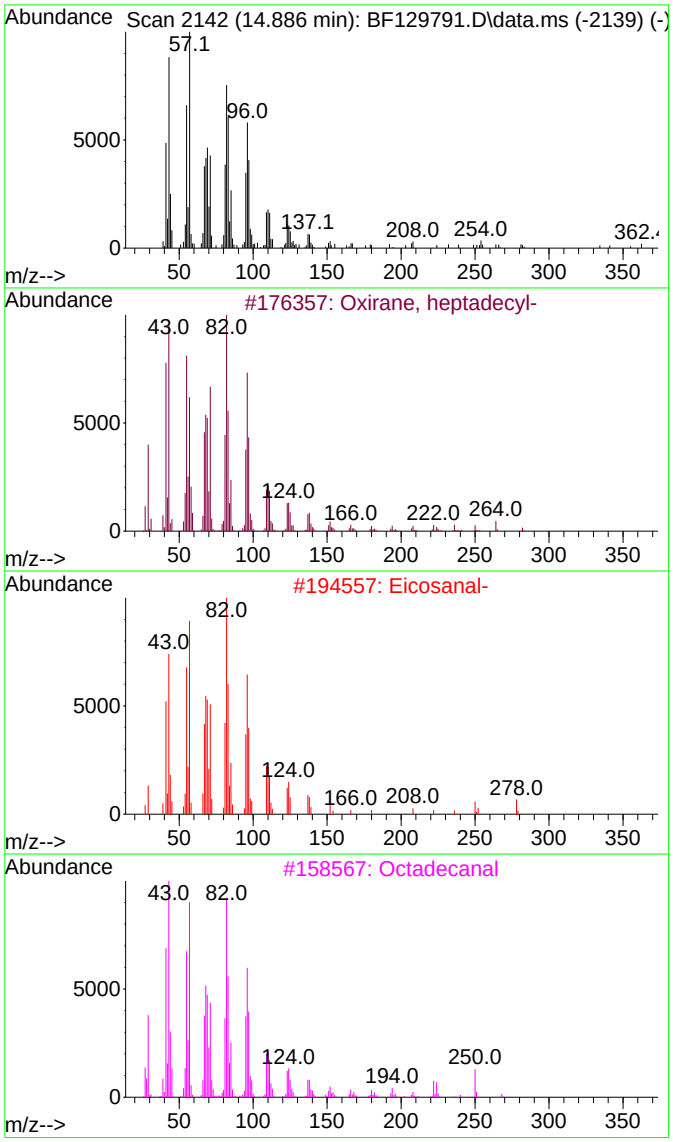
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

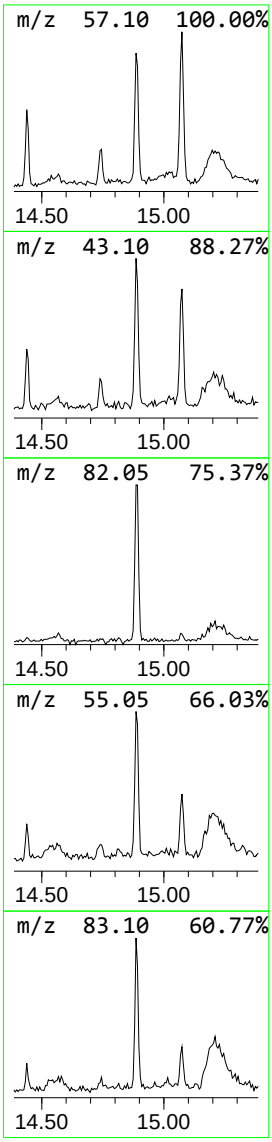
****

Peak Number 3 Oxirane, heptadecyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.886	3.44 ng	147687	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95
2	Eicosanal-	296	C20H40O	002400-66-0	95
3	Octadecanal	268	C18H36O	000638-66-4	91
4	Heptadecanal	254	C17H34O	1000376-70-0	91
5	Hexacosanal	380	C26H52O	026627-85-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081522\
Data File : BF129791.D
Acq On : 15 Aug 2022 20:47
Operator : CG\JU
Sample : N4200-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S9

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

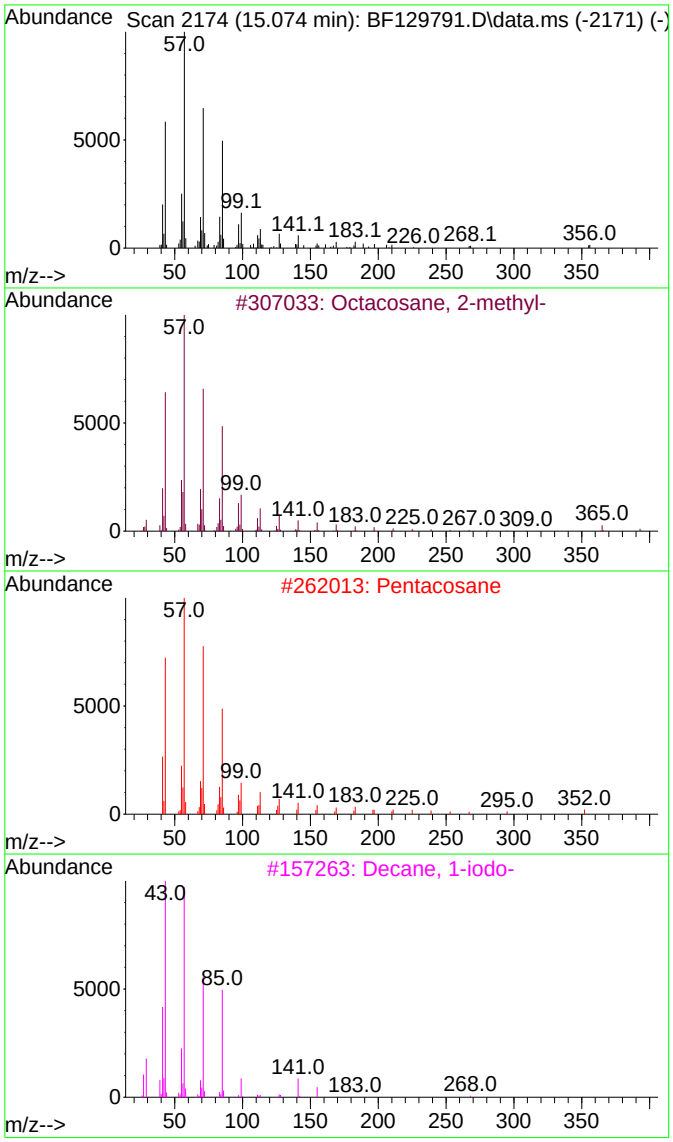
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

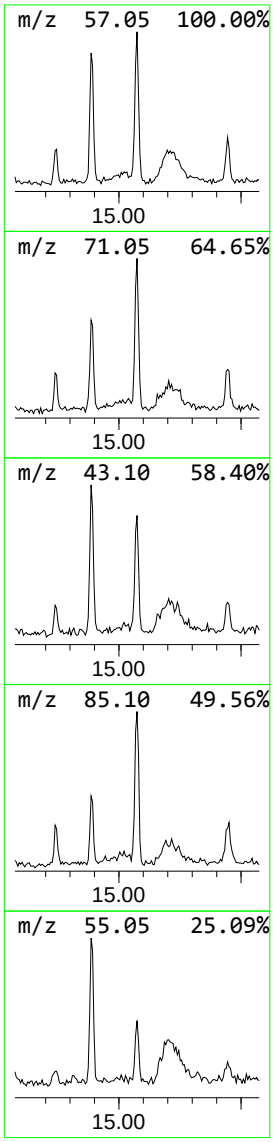
****

Peak Number 4 Octacosane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.074	2.00 ng	86133	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
2	Pentacosane	352	C25H52	000629-99-2	87
3	Decane, 1-iodo-	268	C10H21I	002050-77-3	87
4	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
5	Hexacosane	366	C26H54	000630-01-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081522\
Data File : BF129791.D
Acq On : 15 Aug 2022 20:47
Operator : CG\JU
Sample : N4200-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S9

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
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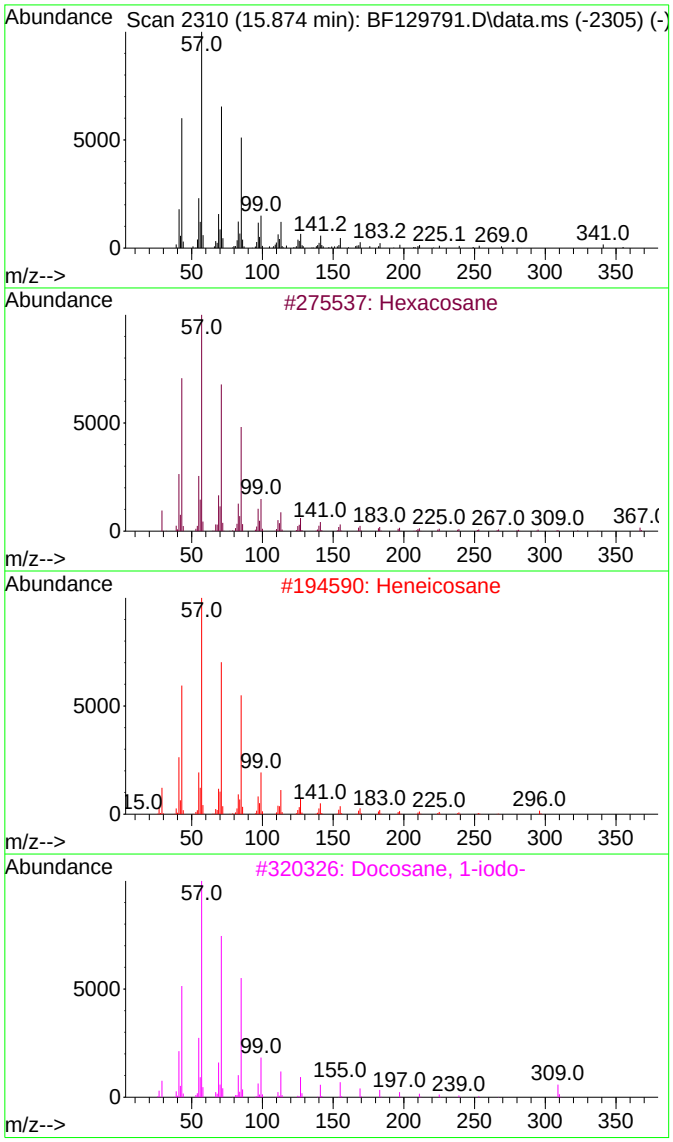
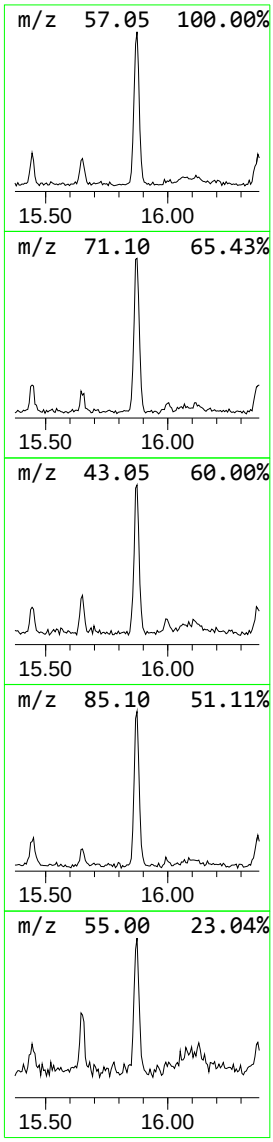
****

Peak Number 5 Hexacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.874	3.82 ng	164055	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





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Sample : N4200-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

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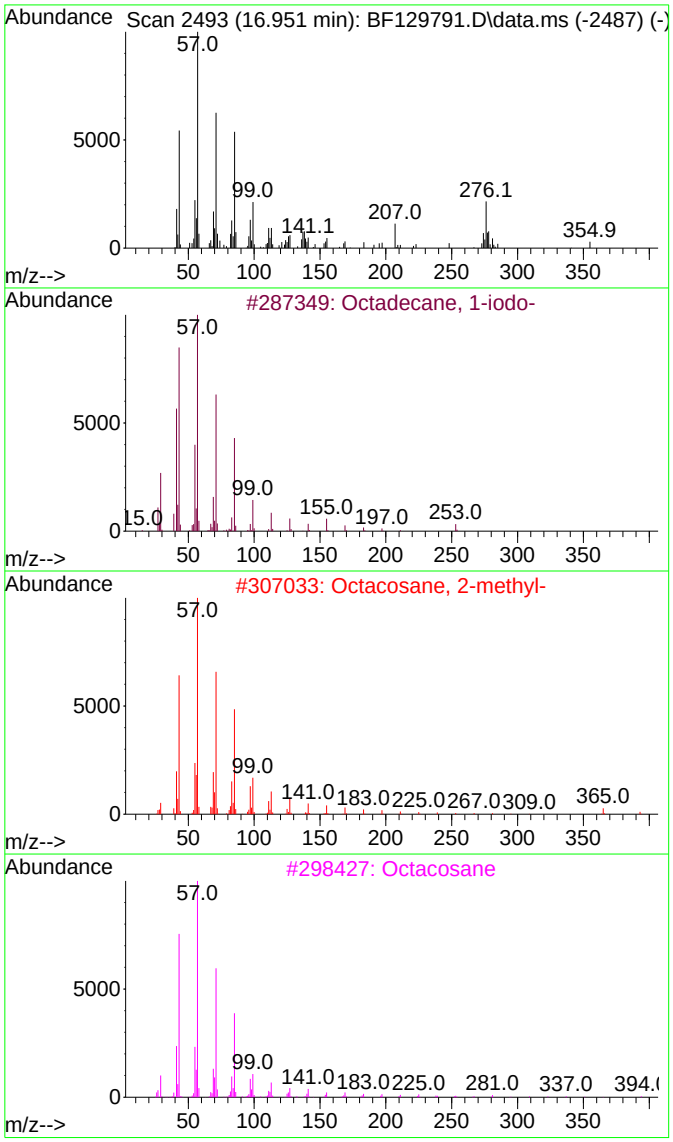
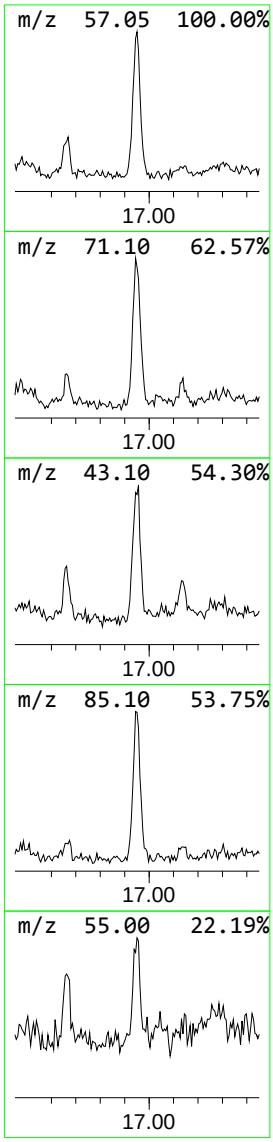
Peak Number 6 Octadecane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.951	2.86 ng	123097	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	58
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	55
3	Octacosane	394	C28H58	000630-02-4	55
4	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	53
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081522\
Data File : BF129791.D
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Operator : CG\JU
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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-...	5.040	18.7	ng	871304	1	6.822	933731	20.0
Dichloroacetic ...	13.886	3.3	ng	176623	5	13.998	1078330	20.0
Oxirane, heptad...	14.886	3.4	ng	147687	6	15.468	859772	20.0
Octacosane, 2-m...	15.074	2.0	ng	86133	6	15.468	859772	20.0
Hexacosane	15.874	3.8	ng	164055	6	15.468	859772	20.0
Octadecane, 1-i...	16.951	2.9	ng	123097	6	15.468	859772	20.0