LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100223\
Data File : BF135529.D
Acq On : 02 Oct 2023 16:06
Operator : CG\JU
Sample : 04672-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-208

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135529.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.381	556	560	577	rBV	3373170	3361230	99.50%	12.025%
2	6.392	728	732	751	rBV	3303042	3378169	100.00%	12.085%
3	6.581	761	764	777	rBV	112438	146031	4.32%	0.522%
4	6.739	788	791	801	rBV	1185988	1056263	31.27%	3.779%
5	7.304	883	887	900	rBV	2017534	2192193	64.89%	7.843%
6	8.022	1004	1009	1021	rBV	1462426	1364362	40.39%	4.881%
7	9.098	1187	1192	1195	rBV	3745061	3311096	98.01%	11.845%
8	9.216	1208	1212	1217	rBV	236375	207948	6.16%	0.744%
9	9.775	1301	1307	1311	rBV	1621227	1402913	41.53%	5.019%
10	10.569	1438	1442	1446	rBV	1927424	1863851	55.17%	6.668%
11	10.698	1459	1464	1470	rVB4	22102	38025	1.13%	0.136%
12	11.269	1557	1561	1564	rBV	1593173	1362805	40.34%	4.875%
13	11.292	1564	1565	1569	rVB	175782	112651	3.33%	0.403%
14	11.669	1625	1629	1635	rBV2	43836	49284	1.46%	0.176%
15	11.774	1644	1647	1648	rBV	48155	39815	1.18%	0.142%
16	11.804	1648	1652	1663	rVB2	560579	601586	17.81%	2.152%
17	11.886	1663	1666	1668	rBV2	54854	49682	1.47%	0.178%
18	12.327	1737	1741	1743	rBV2	44533	48817	1.45%	0.175%
19	12.374	1743	1749	1754	rVV3	96825	139932	4.14%	0.501%
20	12.421	1754	1757	1760	rVB2	43741	44717	1.32%	0.160%
21	12.486	1765	1768	1772	rBV	445558	426803	12.63%	1.527%
22	12.592	1783	1786	1791	rBV3	122345	142990	4.23%	0.512%
23	12.716	1802	1807	1813	rBV	455501	503824	14.91%	1.802%
24	12.768	1813	1816	1821	rVB3	27571	44932	1.33%	0.161%
25	12.863	1828	1832	1835	rBV	2593887	2298574	68.04%	8.223%
26	12.939	1842	1845	1851	rBV3	35705	54984	1.63%	0.197%
27	13.027	1857	1860	1862	rBV3	30923	39139	1.16%	0.140%
28	13.051	1862	1864	1867	rVB2	56928	55319	1.64%	0.198%
29	13.098	1868	1872	1873	rBV	39578	37526	1.11%	0.134%
30	13.157	1879	1882	1889	rVB2	53536	66212	1.96%	0.237%
31	13.439	1926	1930	1933	rBV2	47382	54062	1.60%	0.193%
32	13.568	1950	1952	1956	rVB	38918	36724	1.09%	0.131%
33	13.674	1967	1970	1973	rBV2	51123	54405	1.61%	0.195%
34	13.780	1984	1988	1998	rVB4	120666	221955	6.57%	0.794%
35	13.927	2006	2013	2016	rBV2	912893	984428	29.14%	3.522%
36	13.951	2016	2017	2022	rVB	180796	143251	4.24%	0.512%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100223\
Data File : BF135529.D
Acq On : 02 Oct 2023 16:06
Operator : CG\JU
Sample : 04672-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-208

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.092	2038	2041	2045	rBV2	56443	71111	2.11%	0.254%
38	14.398	2087	2093	2096	rBV2	68994	86333	2.56%	0.309%
39	14.698	2142	2144	2148	rVB	62651	58432	1.73%	0.209%
40	14.968	2186	2190	2198	rBV	137065	274949	8.14%	0.984%
41	15.033	2198	2201	2205	rVB2	79368	91529	2.71%	0.327%
42	15.268	2237	2241	2248	rVB	90685	121583	3.60%	0.435%
43	15.333	2248	2252	2256	rBV	93468	119621	3.54%	0.428%
44	15.392	2257	2262	2274	rVB	692113	951383	28.16%	3.404%
45	15.845	2334	2339	2344	rVB2	56322	83766	2.48%	0.300%
46	16.874	2510	2514	2521	rBV3	44283	89651	2.65%	0.321%
47	17.321	2588	2590	2598	rVB	38987	67514	2.00%	0.242%

Sum of corrected areas: 27952370

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100223\
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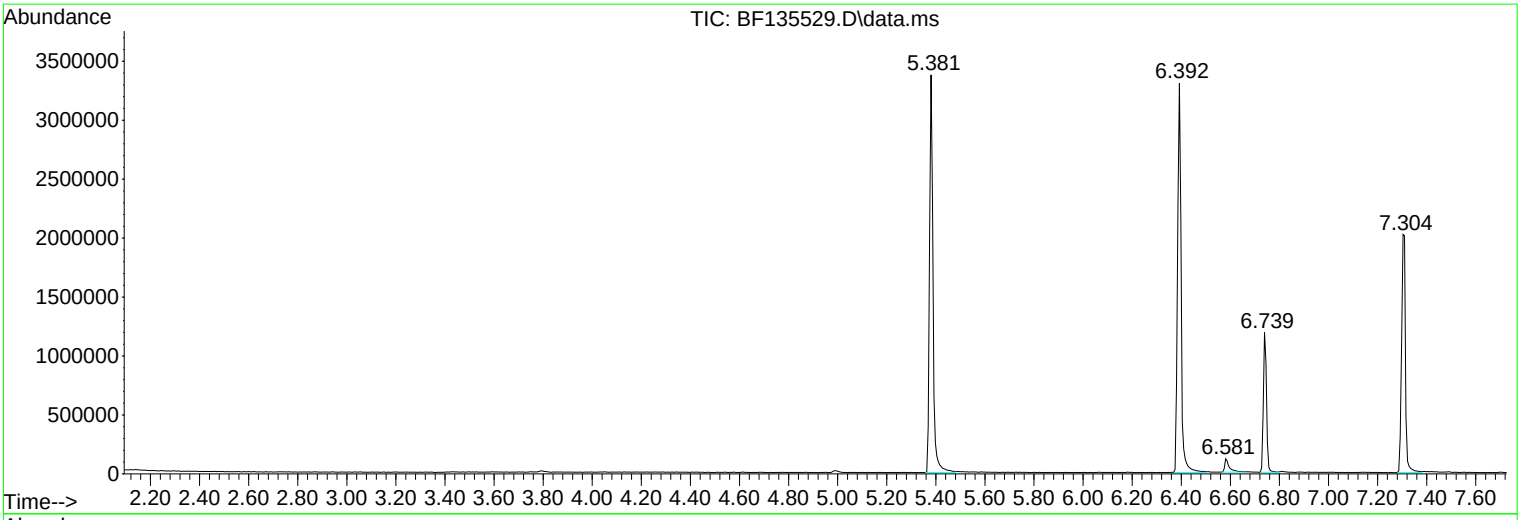
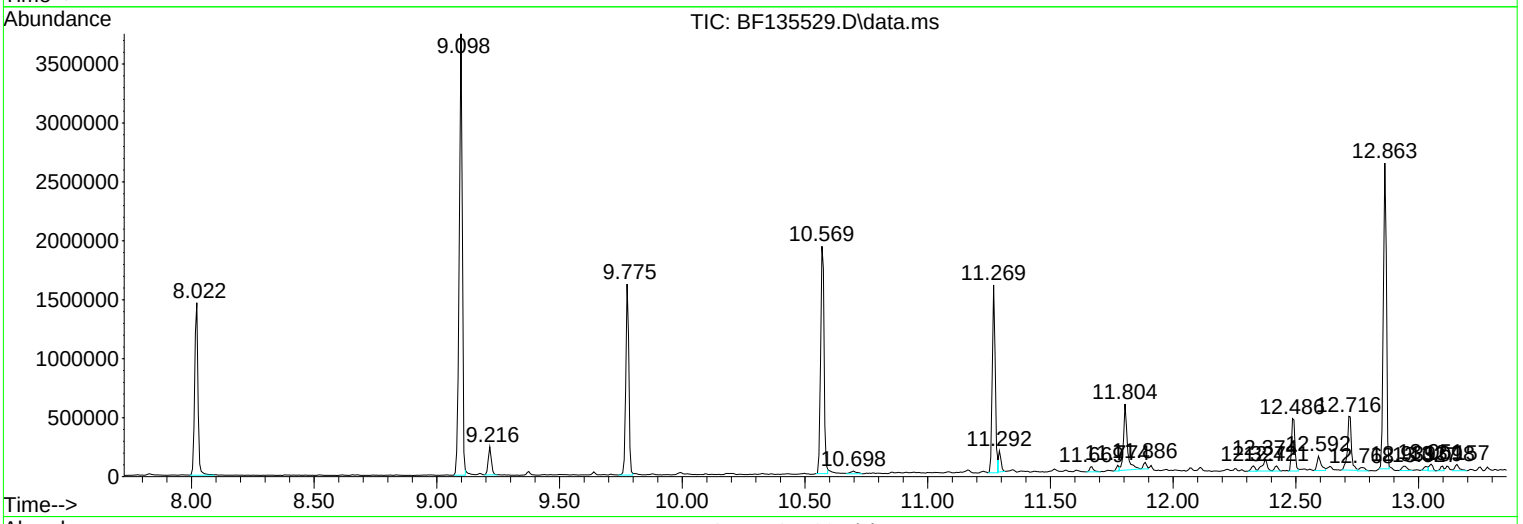
Sample : 04672-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

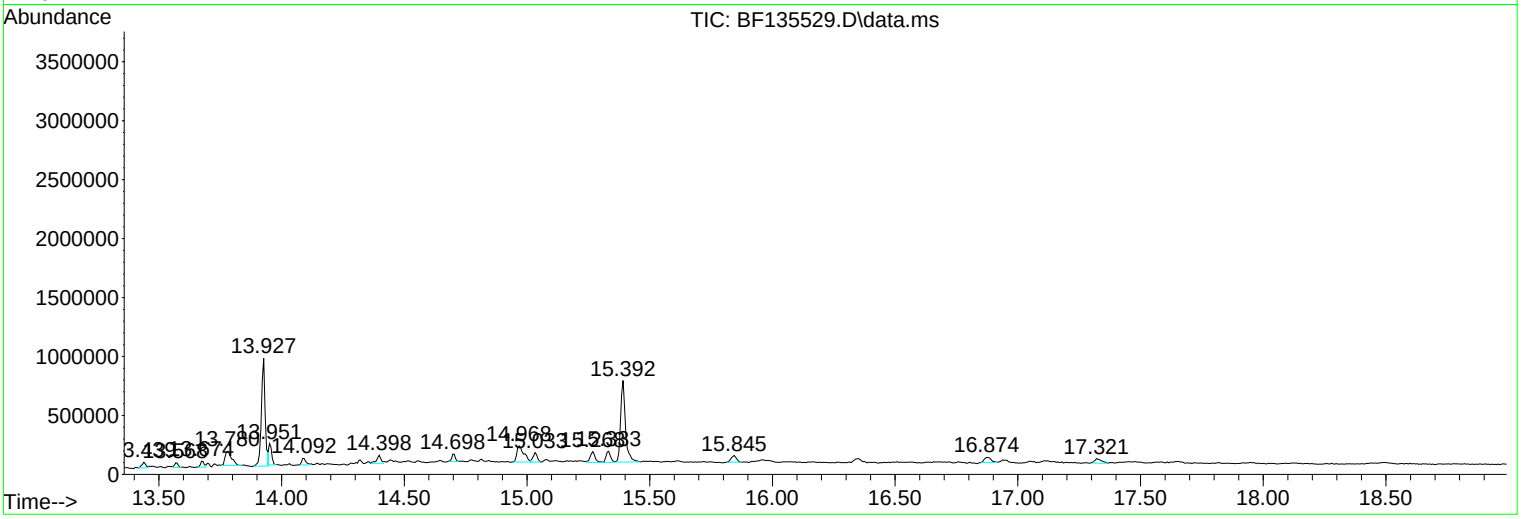
Instrument :
BNA_F
ClientSampleId :
VNJ-208

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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\BF100223\
Data File : BF135529.D
Acq On : 02 Oct 2023 16:06
Operator : CG\JU
Sample : 04672-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-208

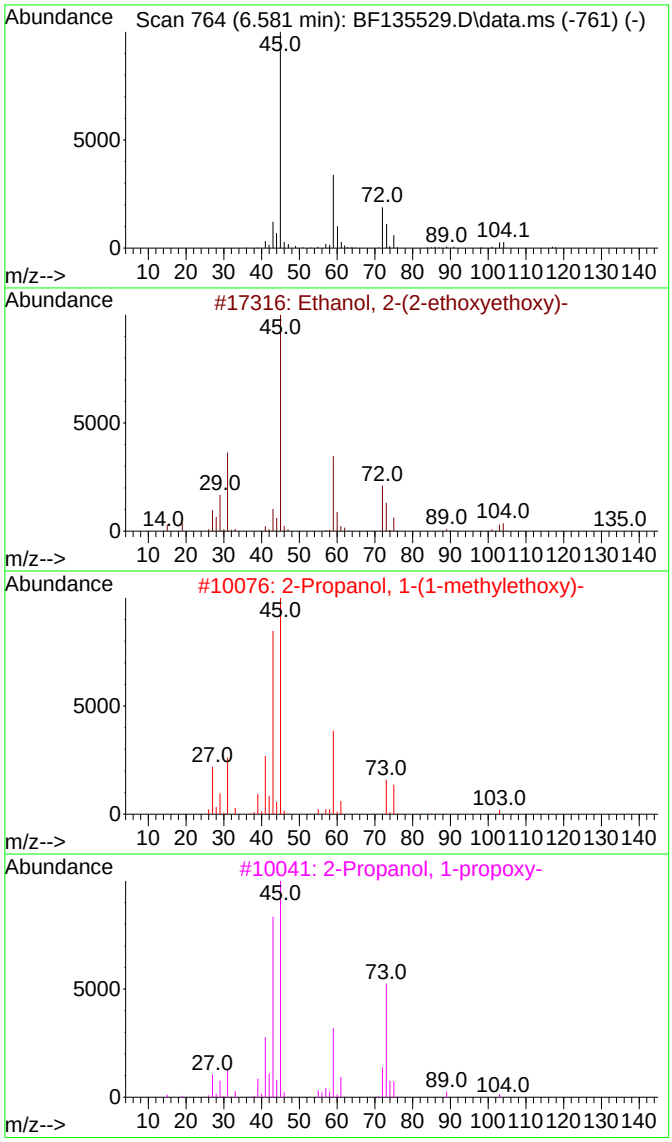
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

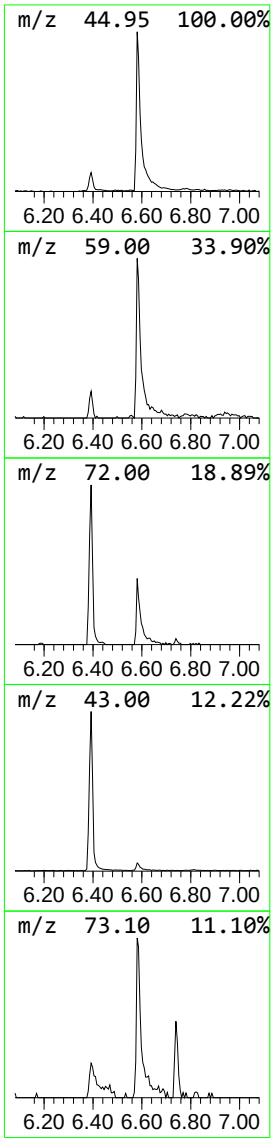
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.581	2.77 ng	146031	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	50
3	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	39
4	Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	38
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100223\
Data File : BF135529.D
Acq On : 02 Oct 2023 16:06
Operator : CG\JU
Sample : 04672-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-208

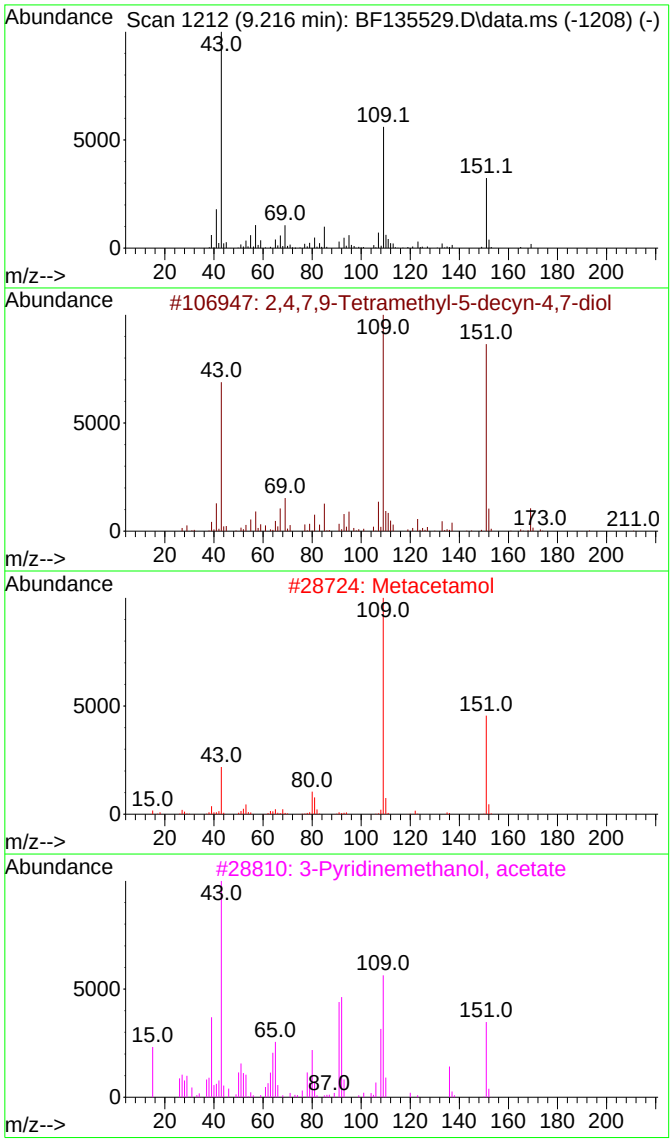
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

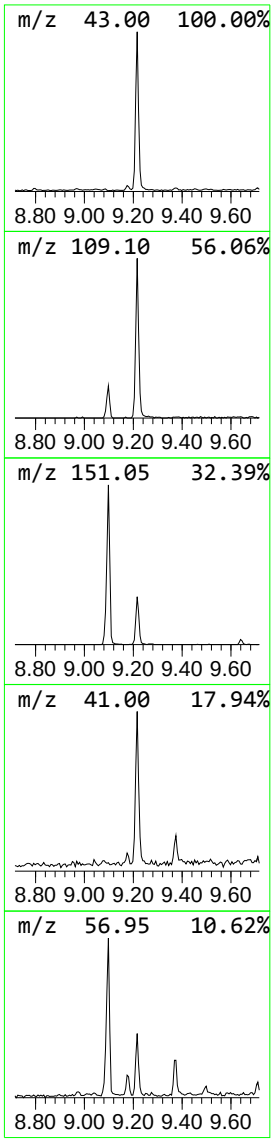
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.216	2.96 ng	207948	Acenaphthene-d10	9.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90
2	Metacetamol	151	C8H9NO2	000621-42-1	47
3	3-Pyridinemethanol, acetate	151	C8H9NO2	010072-09-0	47
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	47
5	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100223\
Data File : BF135529.D
Acq On : 02 Oct 2023 16:06
Operator : CG\JU
Sample : 04672-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-208

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

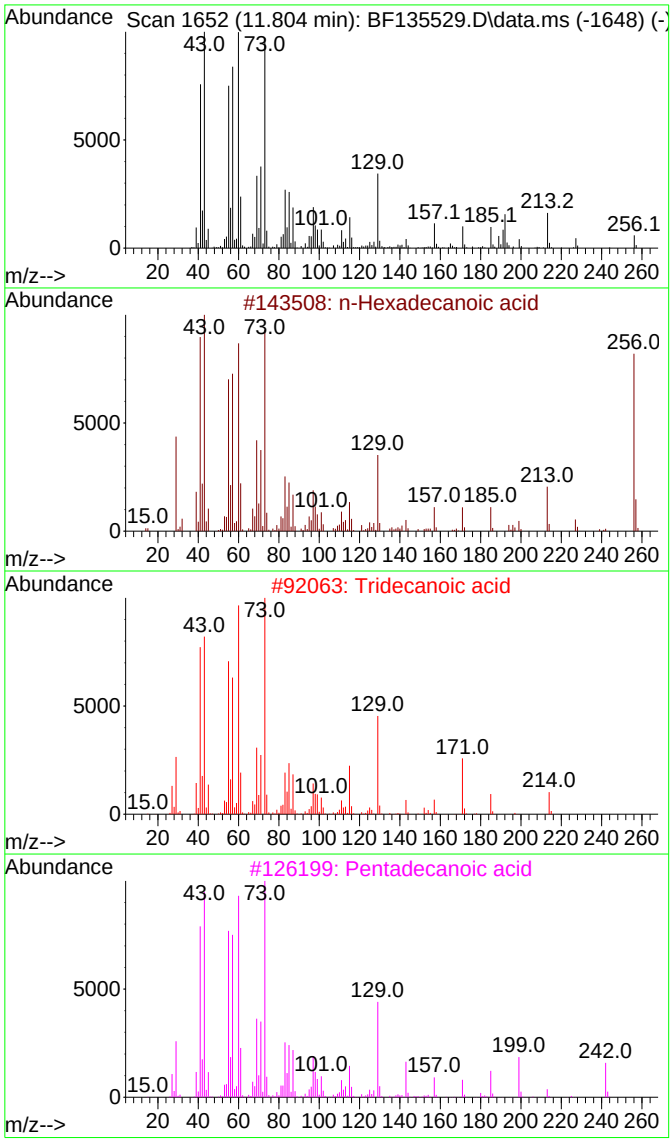
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

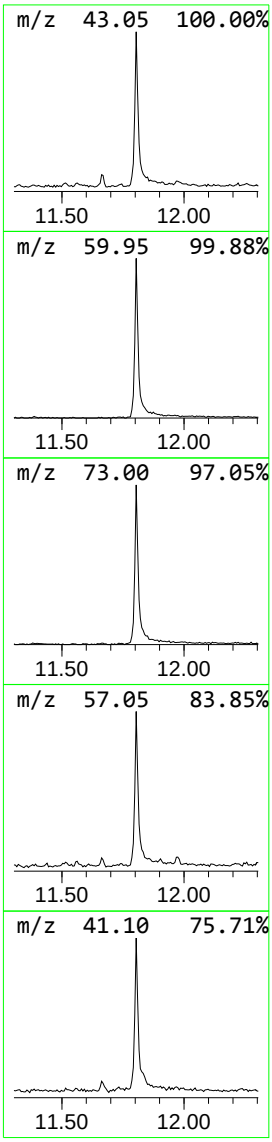
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	8.83 ng	601586	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100223\
Data File : BF135529.D
Acq On : 02 Oct 2023 16:06
Operator : CG\JU
Sample : 04672-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-208

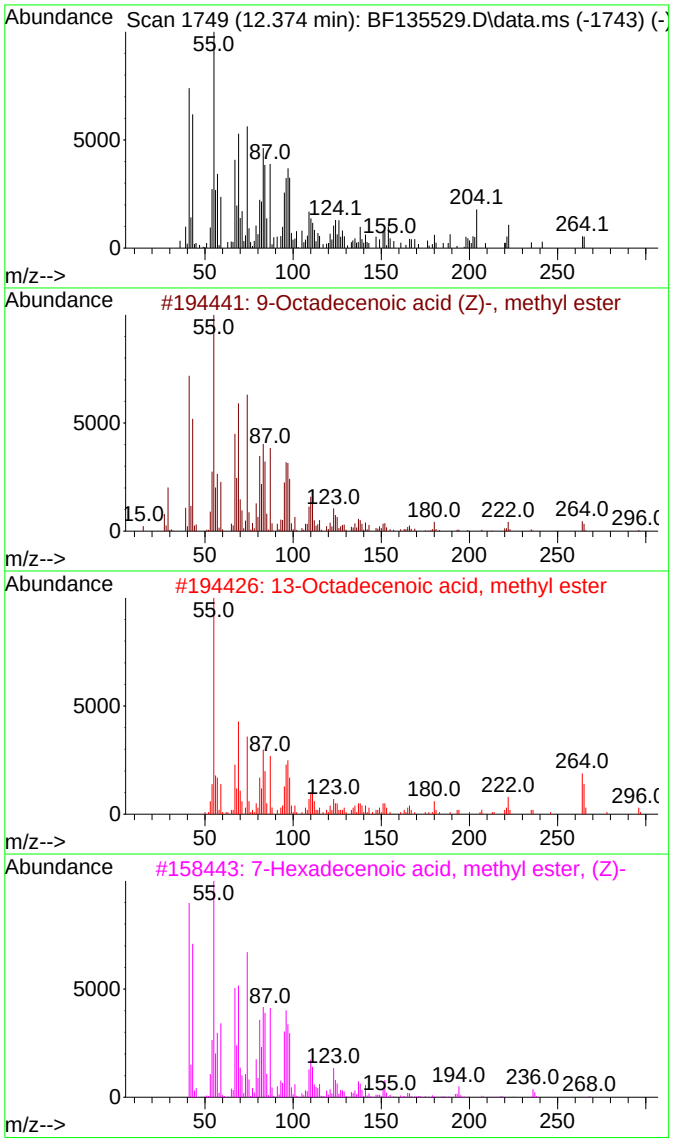
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

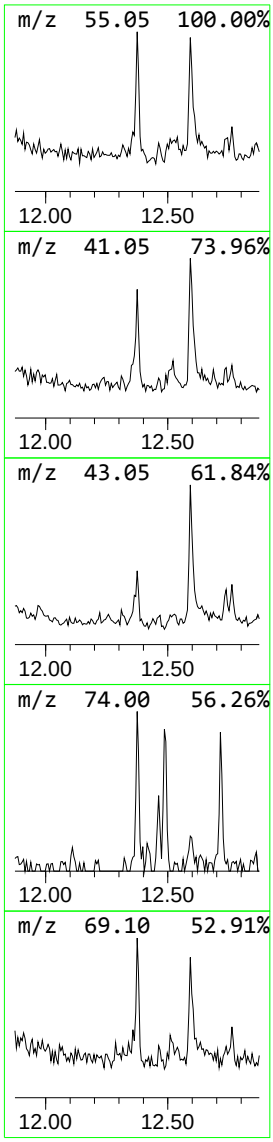
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.374	2.05 ng	139932	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
3	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	90
4	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	90
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100223\
Data File : BF135529.D
Acq On : 02 Oct 2023 16:06
Operator : CG\JU
Sample : 04672-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-208

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

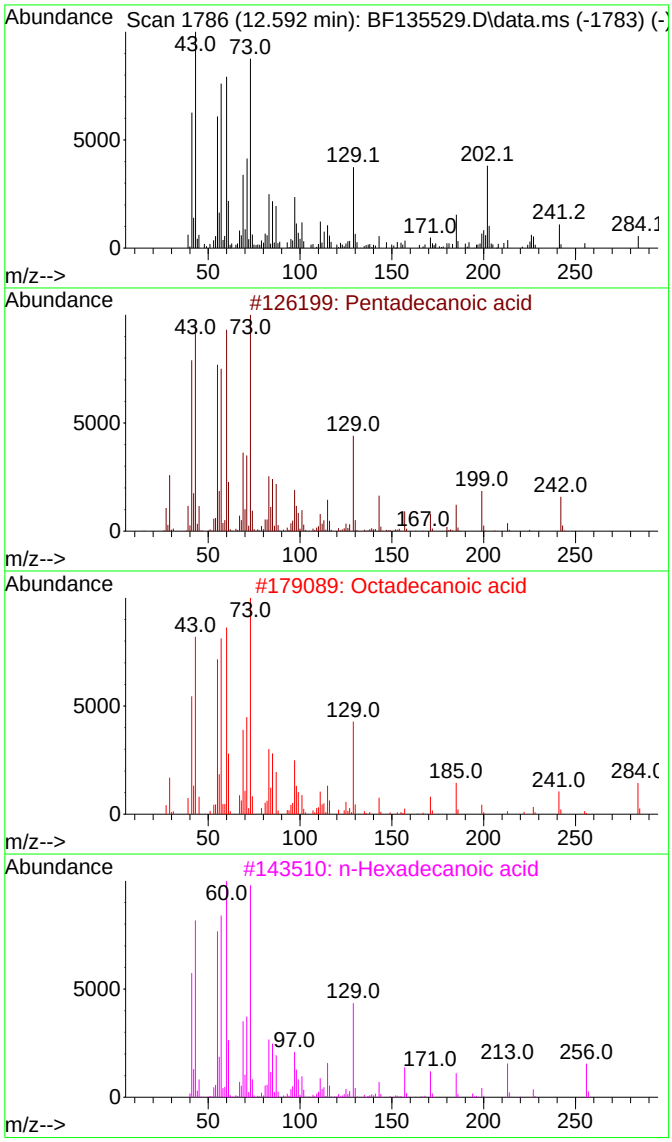
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

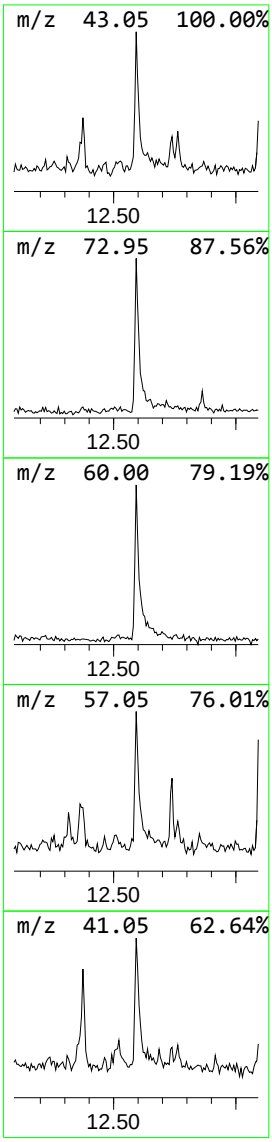
****

Peak Number 5 Pentadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.592	2.10 ng	142990	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2	Octadecanoic acid	284	C18H36O2	000057-11-4	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Dodecanoic acid	200	C12H24O2	000143-07-7	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Data File : BF135529.D
Acq On : 02 Oct 2023 16:06
Operator : CG\JU
Sample : 04672-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-208

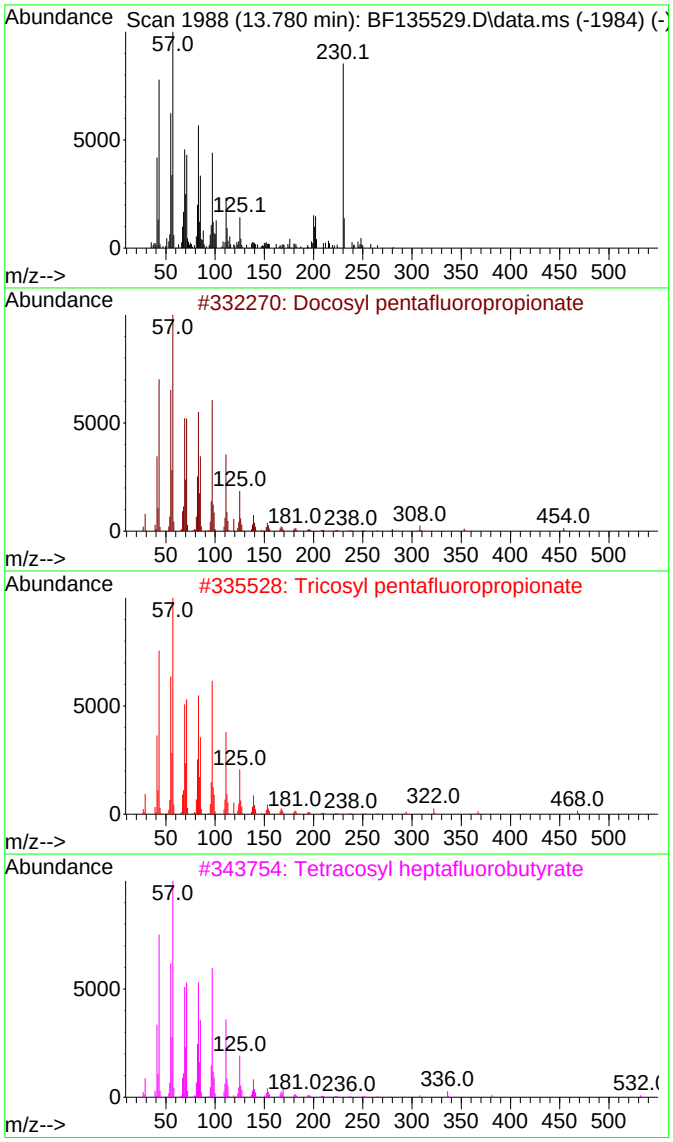
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

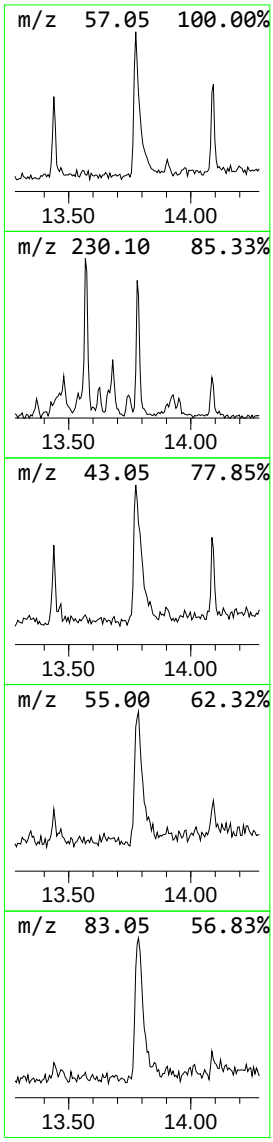
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Docosyl pentafluoropropionate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	4.51 ng	221955	Chrysene-d12	13.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	55
2	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	55
3	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	55
4	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	55
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	55





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Operator : CG\JU
Sample : 04672-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-208

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

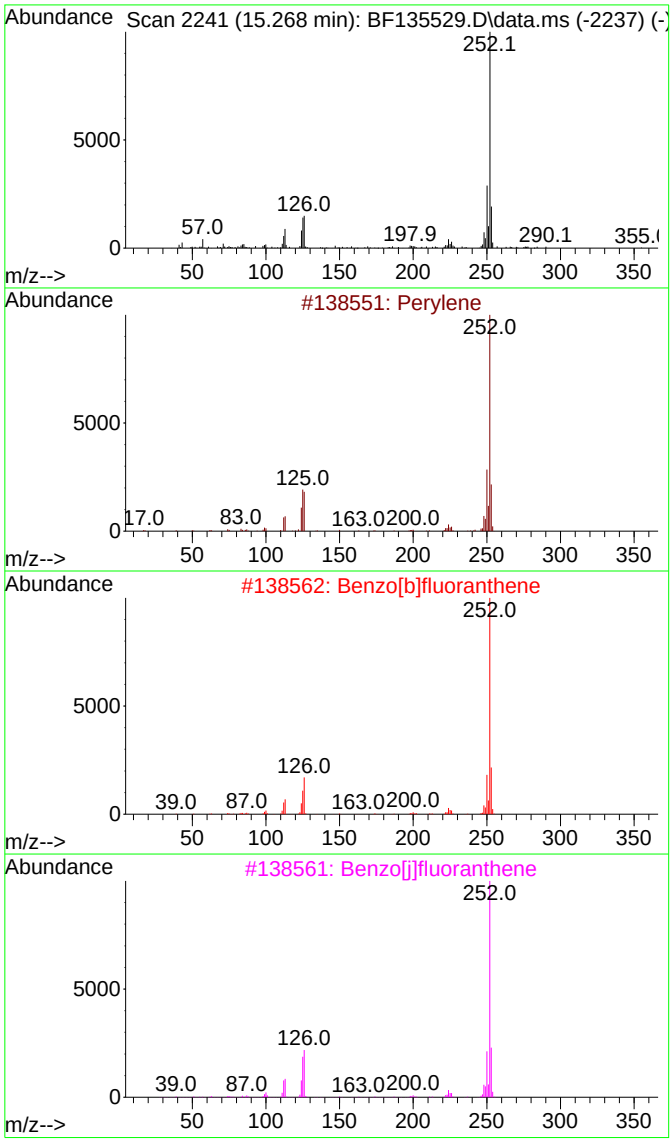
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

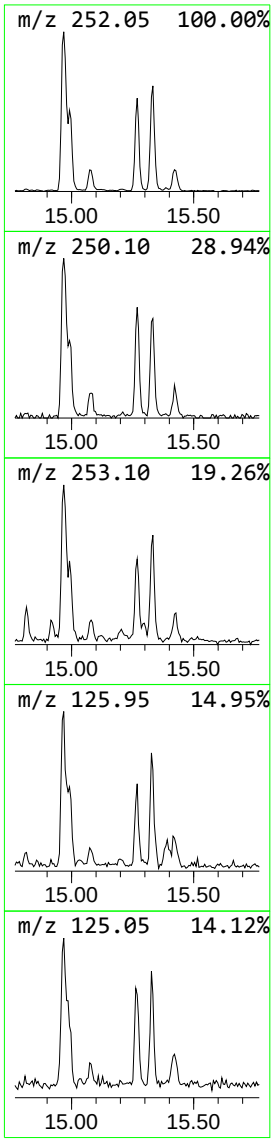
****

Peak Number 7 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.268	2.56 ng	121583	Perylene-d12	15.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	99
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	98
4	Benzo[e]pyrene	252	C20H12	000192-97-2	98
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100223\
Data File : BF135529.D
Acq On : 02 Oct 2023 16:06
Operator : CG\JU
Sample : 04672-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-208

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
Ethanol, 2-(2-e...	6.581	2.8	ng	146031	1	6.739	1056260	20.0
2,4,7,9-Tetrame...	9.216	3.0	ng	207948	3	9.775	1402910	20.0
n-Hexadecanoic ...	11.804	8.8	ng	601586	4	11.269	1362810	20.0
9-Octadecenoic ...	12.374	2.0	ng	139932	4	11.269	1362810	20.0
Pentadecanoic acid	12.592	2.1	ng	142990	4	11.269	1362810	20.0
Docosyl pentafl...	13.780	4.5	ng	221955	5	13.927	984428	20.0
Perylene	15.268	2.6	ng	121583	6	15.392	951383	20.0